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Expanded HD Ton Container Solid Heel Modeling

Report 05007

Revision 0

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Prepared for

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EXECUTIVE SUMMARY

The Tooele Chemical Destruction Facility (TOCDF) is preparing to destroy their stockpile of ton containers holding agent HD. Sampling and analysis by TOCDF of these HD ton containers has been completed. Analysis results indicated that agent within a number of the ton containers has concentrations of Site Specific Risk Assessment Metals such as mercury (Hg). The feed rate to the Metal Parts Furnace (MPF) and Liquid Incinerator (LIC) for agent containing these metals may have to be reduced in order to maintain compliance with emissions limits. Additionally, ultrasonic and x-ray testing indicate that a large portion of the ton containers have solid residues that will prevent them from being drained to a 5% residual agent heel.

Continental Research and Engineering, LLC (CR&E) has completed an evaluation of processing HD ton containers having solid heels. A numerical model was created utilizing the Fluent Computational Fluid Dynamics (CFD) program. The CFD model simulates the heating, melting and vaporization of agent solids in combination with liquid agent. Agent solid and liquid properties input to the CFD model utilized the properties measured by sampling and analysis of the TOCDF HD ton container stockpile.

The output from the CFD vaporization model was used as an input to the CR&E mass and energy balance model to predict key furnace operating conditions and processing times required for the TOCDF HD ton containers. Furnace processing conditions, minimum feed rate and the required minimum residence times required for processing TOCDF HD Ton Containers with various solid heel depths were calculated. All cases investigated predict that processing can be completed well within the capabilities of the furnace system while maintaining permitted furnace operating conditions. The recommended tray feed intervals and total furnace residence times required for processing of TOCDF ton containers with varying depths of solid agent heel are shown in Table 1.

Table 1: Tray Feed Intervals and "5X" Minimum Residence Times
for TOCDF HD Ton Containers with Varying Solid Heels

MPF Operating at 1,450°F							
	1-Inch Solid HD	2-Inch Solid HD	3-Inch Solid HD	4-Inch Solid HD	5-Inch Solid HD	6-Inch Solid HD	7-Inch Solid HD
Tray Feed Interval [minutes]	31	41	59	79	91	104	116
Minimum 5X Residence Time [minutes]	84	102	122	146	162	180	196
MPF Operating at 1,600°F							
Tray Feed Interval [minutes]	24	36	52	67	77	88	98
Minimum 5X Residence Time [minutes]	72	86	106	122	136	152	164

It is recommended that the water spray nozzles in the top of furnace Zones 1 and 2 be changed to a vertical downward orientation in order to aid in furnace temperature control during processing of the HD ton containers.

Smoking as they exit from the discharge airlock is not anticipated to be a problem for ton containers with HD agent.

INTRODUCTION AND BACKGROUND

The MPF is one of three furnace systems utilized by the Continental United States (CONUS) baseline chemical demilitarization facilities to incinerate or decontaminate chemical agents and munitions. Projected MPF throughput rates assumed the munitions could be drained to a 5% residual agent heel. Based on Johnston Atoll Chemical Agent Disposal System (JACADS) experience, this assumption may be optimistic for mustard filled munitions and bulk containers. The presence of partially or totally solidified agent in mustard munitions prohibited draining of munitions and lengthened processing times at JACADS.

Further, metal contaminants in mustard agents may be a significant limiting factor in the throughput of munitions to the MPF. Sampling and analytical data from HD ton containers in the TOCDF stockpile indicate that agent within some of the containers have concentrations of Site Specific Risk Assessment Metals such as mercury. The feed rate to the MPF and LIC for agent containing mercury and other metals may have to be reduced in order to maintain compliance with emissions limits.

Ultrasonic testing and limited x-ray testing of the HD ton containers has also been completed. A large number of the ton containers were found to contain solids that will prevent them from being drained to a 5% residual agent heel.

CR&E utilized numerical model simulations to predict agent vaporization from HD ton containers holding varying quantities of solids and liquid agent mixed together. The predicted agent vaporization rates were then used as input to the CR&E MPF mass and energy balance calculations to predict furnace operating conditions and throughput rates.

A numerical model was created utilizing the Fluent Computational Fluid Dynamics (CFD) program to simulate the processing of HD ton containers having a mix of solid and liquid agent. The CFD model simulates the heating, melting and vaporization of agent solids in combination with liquid agent vaporization. Agent parameters input to the CFD model utilized the properties measured by sampling and analysis of the TOCDF HD ton container stockpile. Performance of the CFD model was previously verified by comparing results to vaporization rates from the CR&E Peak Vaporization Rate (PVR) model and plant processing data for liquid agent VX. Agent VX was used because it was the only agent for which actual processing data was available.

CR&E has developed mass and energy (M&E) balance models of the MPF to predict furnace performance during munitions processing. The model is a spreadsheet calculation for mass flows and energy balance calculated at 30-second intervals using a quasi steady-state assumption. Inputs to the model include agent vaporization rate from the CR&E Peak Vaporization Rate model, and/or the CR&E CFD vaporization model, furnace air flows, heat losses and furnace temperature. The spreadsheet calculates furnace conditions for each time interval.

The output from the CFD vaporization model was used as an input to the mass and energy balance model to predict key furnace operating conditions and processing times required for the TOCDF HD ton containers. Furnace processing conditions, minimum feed rate and the required minimum residence times required for processing TOCDF HD ton containers with various solid heel depths were calculated.

The CFD vaporization calculations initially used an MPF operating temperature of 1,450°F. The simulations were then repeated, using a temperature of 1,600°F, in order to determine if higher operating temperatures will enhance TOCDF container processing operations.

ANALYSIS

HD Agent Characterization for Ton Containers at TOCDF

H mustard was manufactured at Rocky Mountain Arsenal (RMA) using the Levinstein process. American Levinstein (H) mustard was produced by reacting dry ethylene with sulfur monochloride. The H produced contained a high percentage of sulfur impurities, was found to be unstable, and tended to deteriorate in bulk storage and in filled munitions.

A water wash process followed by vacuum distillation was developed to remove most of the impurities in H mustard and produce a more stable product called HD. A water wash/distillation facility was constructed at Rocky Mountain Arsenal (RMA) for production of HD. The ton containers residing at TOCDF/Deseret Chemical Depot (DCD) were filled with agent produced at RMA. The chemical characteristics of HD at time of manufacture are summarized in Table 2.

Table 2: Chemical Composition of Distilled Mustard Agent When Manufactured

Chemical Compounds	wt %
Bis (2-chloroethyl) sulfide {HD}	92
Free sulfur	7.38
Ferric chloride	0.5
Hydrochloric acid	0.11

Composition of the agent is expected to undergo chemical and physical changes as it ages by amounts that will vary between munitions, point of manufacture, and storage history. The HD has been found to react during storage and ultimately form a solid heel.

Intrusive sampling of 98 HD ton containers from the inventory at TOCDF/DCD was accomplished between January and May 2003. The agent samples were transported to the Edgewood Chemical Biological Center for analysis. Liquid and solids sample compositions were determined.

Analyses of the solidified residue showed that it was composed of Agent HD and a number of compounds formed by the breakdown of Agent HD. The mass of Agent HD was reported to be no greater than 47 wt% of the total solidified material. A majority of the remaining material was composed of two Agent HD breakdown products; S-(2-chloroethyl)-1, 4-dithianium with a range of 17.6 wt% to 36.9 wt% and 1,4-dithioniabicyclo[2.2.2] octane with a range of 6.3 wt% to 17.6 wt%.

The available analyses for samples of Agent HD presents limited results for inorganic compounds. When inorganic/metals analysis was performed on a sample, the iron (Fe) content was generally higher than for other constituents tested for on a parts per million by weight basis. The relative magnitude of the mass of the Fe in comparison to the total mass of the agent, however, was not reported. Fe and other inorganic compounds were excluded from the assumed composition utilized for model construction since it was not possible to determine a reasonable estimate of the mass of these components present.

A set of liquid HD and HD solid residue properties were developed from the composition analyses of these materials available. These properties were utilized as input to the CFD vaporization model. Noninvasive testing of the total ton container inventory at TOCDF/DCD was accomplished between July and September, 2002 utilizing ultrasonic testing. Agent fill levels averaged 23 inches and solids heel levels averaged 4.27 inches. No correlation was apparent between agent fill and solids heel levels or between different production lots.

Limited x-ray data has recently been gathered for some of the ton containers in the TOCDF/DCD inventory. This data provides a profile of the solid heel present within the ton containers and a measurement of the total solid heel volume.

A profile of the solid heel was developed for modeling from the available noninvasive testing completed (see Figures 1 and 2). A series of solid heel depths (from 1 inch to 7 inches) were modeled since there was a large discrepancy in solids depth measured by the two methods used for solid heel measurement. A residual liquid agent depth of 2 inches over the top of the solid heel was modeled for all cases.

Ton Container Computational Fluid Dynamics Model

Computational Fluid Dynamics modeling was utilized to predict the rate of agent melting and vaporization for a mixed solid/liquid heel contained in a Ton Container during processing through the Metal Part Furnace.

CFD Physical Model

In addition to the fundamental equations, such as the continuity, energy, and Navier-Stokes equations, models must be employed for accurate results. The non-linear (NL) k-ε turbulence model and Discrete Ordinates (DO) radiation model were used in this project. The DO radiation model solves the radiation heat transfer problems using a finite number of angles from each heat source. The advantage of the DO model is moderate computational cost and memory requirements.

The transport equations for momentum, k and ε:

$$\frac{\partial}{\partial x_j}(\rho U_i U_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}[\mu(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}) - \rho\overline{u_i u_j}] \quad (1)$$

$$\frac{\partial}{\partial x_i}(\rho U_i k) = \frac{\partial}{\partial x_i}(\alpha\mu_{eff}\frac{\partial k}{\partial x_i}) + \mu_{eff}S^2 - \rho\varepsilon \quad (2)$$

$$\frac{\partial}{\partial x_i}(\rho U_i \varepsilon) = \frac{\partial}{\partial x_i}(\alpha\mu_{eff}\frac{\partial \varepsilon}{\partial x_i}) + C_{\varepsilon 1}\frac{\varepsilon}{k}\mu_t S^2 - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} - \rho R \quad (3)$$

DO radiation equation:

$$\frac{d(Is_i)}{dx_i} + (a+\sigma_s)I(r,s) = an^2\frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi}\int_0^{4\pi} I(r,s')\Phi(s\cdot s')d\Omega' \quad (4)$$

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Melting/Vaporization Control Code

The CR&E melting/vaporization control code, coupled with the NL k-ε model and DO radiation model, is used to simulate the melting and/or vaporization process. The Ton Container CFD vaporization model developed by CR&E can simulate the effect of liquid chemical agent mixed with different solid mass fractions within a ton container during processing in the MPF.

Two scalars are used in the vaporization control code. The first scalar is used to measure the solid mass fraction. When the temperature of a computational cell reaches the melting point of the solid component, the solid will begin to melt. The heat flux of the cell is calculated and the solid mass fraction is adjusted accordingly during the heating/melting process. The energy source term in the energy equation and momentum source terms in the k-ε equation are adjusted by the vaporization control code of the model. The temperature of the cell remains at the melting point of the solid until the solid mass fraction in that cell reaches zero.

The liquid mass fraction was measured by the second scalar. The first and the second scalars each perform a similar function in the modeling process. The liquid begins to vaporize when the cell temperature reaches the liquid boiling point. The cell temperature remains at the boiling point until the liquid mass fraction in that cell reaches zero.

Melting/vaporization equation:

$$\frac{d(\rho \forall_{cell} \in_{cell})}{dt} = -\frac{Q_{cell}}{L} \tag{5}$$

Where

ρ is density of agent

$\forall_{cell}$ is numerical cell volume

$\in_{cell}$ is solid / liquid mass fraction of the cell

t is simulation time from solver in second

Q_{cell} is heat flux transfer in the cell boundary

L is Latent heat of solid melting / liquid vaporization

Agent Properties

The properties for agent VX, liquid agent HD and solid HD heel utilized within the model simulations are shown in Tables 3-5. The liquid agent properties are the same as those used in the CR&E PVR model.

Table 3: Ton Container Liquid VX Heel Properties

Parameter	Model Values
Density [lbm/ft^3]	92.77 @ 80°F
Heat Capacity [Btu/lbm·°F]	0.407 @ 80°F
Boiling Point [°F]	568.04
Heat of Vaporization [Btu/lbm]	140.76
Thermal Conductivity [Btu/h·ft·°F]	0.11 @ 80°F

Table 4: Ton Container Liquid HD Heel Properties

Parameter	Model Values
Density [lbm/ft^3]	75.97 @ 80°F
Heat Capacity [Btu/lbm·°F]	0.327 @ 80°F
Boiling Point [°F]	423
Heat of Vaporization [Btu/lbm]	168.71
Thermal Conductivity [Btu/h·ft·°F]	0.079 @ 80°F

Table 5: Ton Container Solid HD Heel Properties

Parameter	Model Values
Density [lbm/ft^3]	98.01
Heat Capacity [Btu/lbm·°F]	0.444
Melting Point [°F]	212
Heat of Fusion [Btu/lbm]	87.075
Boiling Point [°F]	463.7
Heat of Vaporization [Btu/lbm]	285.52
Thermal Conductivity [Btu/h·ft·°F]	0.11

Model Configuration

Seven mass quantities of liquid/solid HD heel contained in a ton container were evaluated. Figure 1 shows the solid heel level outline of ton container number 46992 obtained from X-Ray testing and the averaged solid heel geometry determined for use in the model construction. This geometry was scaled for determination of varying solid heel depths as shown in Figure 2. Dimensions and mass quantities for each solid heel configuration are shown in Table 6. A liquid agent depth of 2 inches over the center solid heel was utilized in all cases.

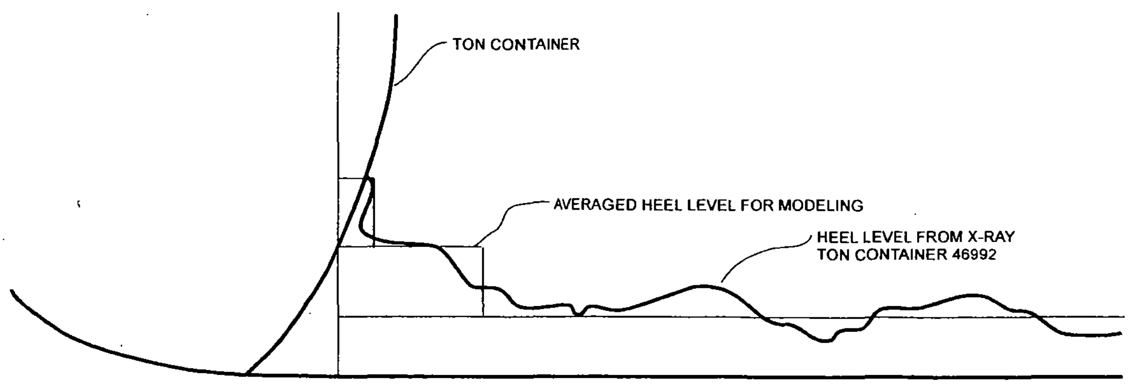


Figure 1: Ton Container no. 46992 Solid Heel Level Obtained from X-Ray data

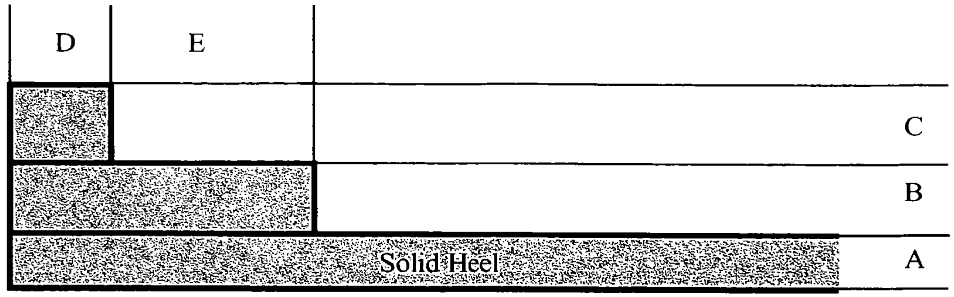


Figure 2: Ton Container Solid Heel End Profile for Varying Center Heel Depth

Table 6: Ton Container CFD Modeling Configurations

Case	Solid HD Heel					Solid HD	Liquid HD
	Center Depth	End Depth		End Width			
	A (in)	B (in)	C (in)	D (in)	E (in)	(lbm)	(lbm)
1" solid with 2" top liquid HD	1	1.1	1.1	0.5	1.5	31.64	87.15
2" solid with 2" top liquid HD	2	2.2	2.2	1	3	100.11	96.47
3" solid with 2" top liquid HD	3	3.3	3.3	1.5	4.5	201.77	102.11
4" solid with 2" top liquid HD	4	4.4	4.4	2	6	335.42	103.9
5" solid with 2" top liquid HD	5	4.4	4.4	2	6	422.13	111.55
6" solid with 2" top liquid HD	6	4.4	4.4	2	6	514.55	117.96
7" solid with 2" top liquid HD	7	4.4	4.4	2	6	611.71	123.32

439.3
534
632

Computational Geometry and Mesh

The CFD model geometry is divided into a series of cells (meshed). The CFD program then performs calculations of heat transfer between the model cells. Mesh size and quality determines the accuracy and stability of the model numerical computations. The attributes associated with mesh quality are node point distribution, smoothness, and skewness. A hexahedral grid was used in meshing of this model. This mesh allows an accurate solution to be obtained with as few cells as possible, making the computational geometry more efficient. It allows a large aspect ratio without increasing skewness, which may impede accuracy and convergence.

The Ton Container model consists of geometry for both liquid and solid chemical agent, the steel wall and ends of the ton container, and the 1-inch thick insulation (Fiberfrax durablanket-S) of the ton container cradle located on the bottom half of the container. Only one half of the ton container was simulated in this study considering the front/back symmetry of the ton container and boundary conditions. This simplified model construction shortened the computational time required. The geometry and mesh of the ton container half with agent HD is illustrated in Figure 3. The geometry of liquid and solid HD heel showing the solid end profile for varying center heel depths is shown in Figure 4.

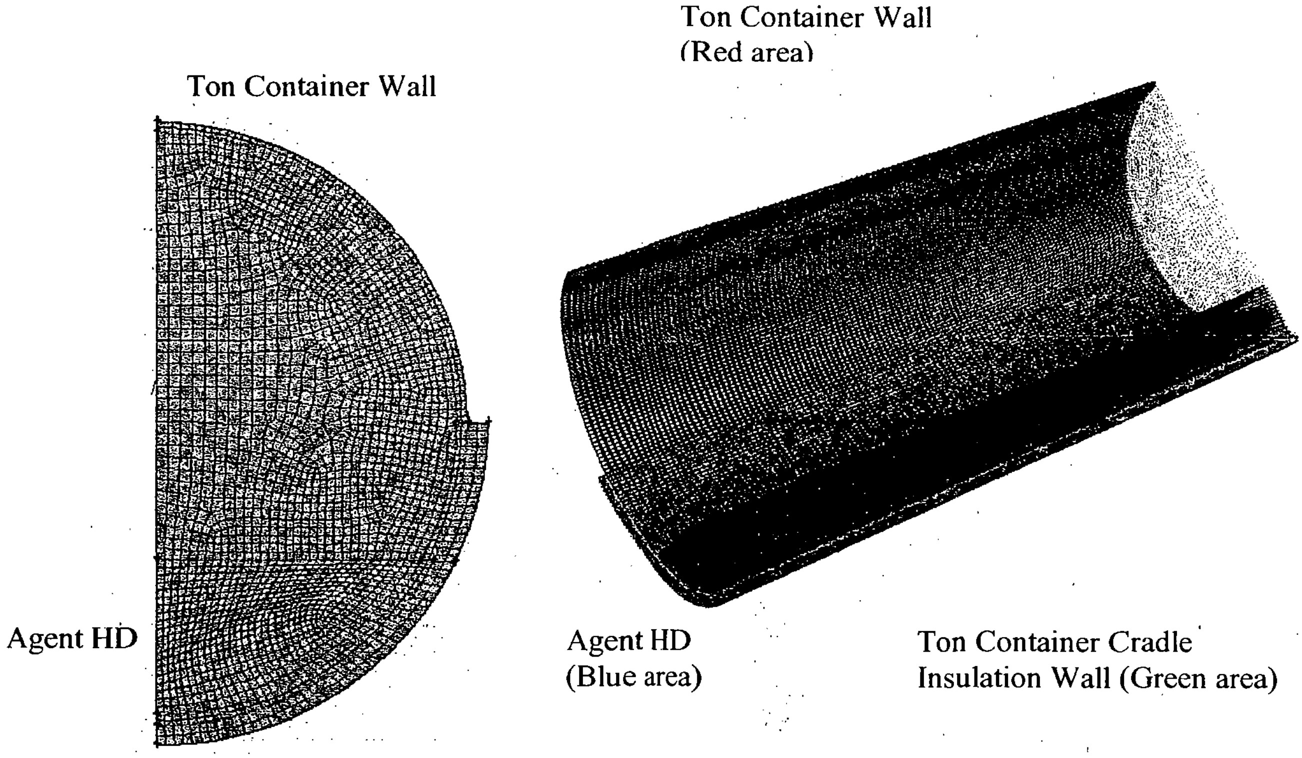
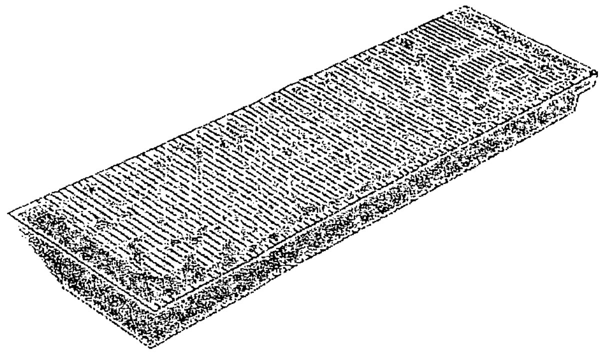
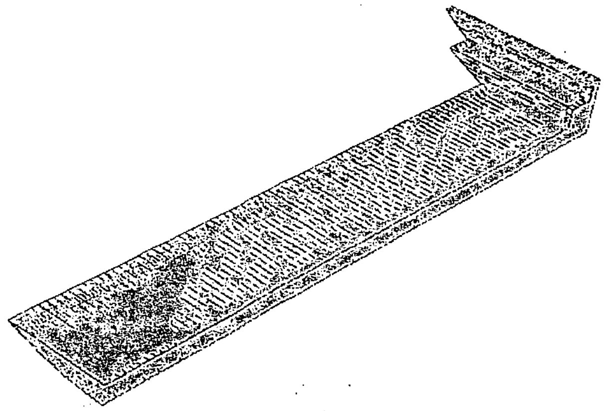


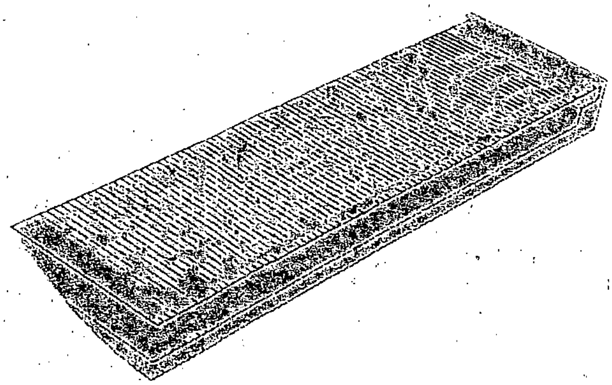
Figure 3: Geometry and Mesh of the Ton Container CFD Model



Liquid HD Heel



Solid HD Heel



Liquid & Solid HD Heel

Figure 4: Geometry and Mesh of the Liquid/Solid Heel in Ton Container

Model Boundary Conditions

Furnace air temperature was set at 1,450°F for the first simulation run and at 1,600°F for the second. The other objects were set at 70°F at the start of both simulations. Air was used as the fluid inside the MPF for heat transfer simulation. The model furnace temperature was controlled to a constant of 1,450°F or 1,600°F, respectively, for the first and second simulations. The material properties for the ton container and furnace walls were set to those of mild steel. The properties set for the Fiberfrax Durablanket-S insulation were as indicated in Table 7.

Table 7: Fiberfrax Durablanket-S Properties

	Temperature (°F)			
	392	752	1,112	1,472
Density [lbm/ft^3]	6.0			
Heat Capacity [Btu/lbm·°F]	272.3			
Thermal Conductivity [Btu/h·ft·°F]	0.029	0.052	0.081	0.127

CFD Model Procedures

The finite-volume method using the SIMPLEC algorithm was utilized to obtain a pressure correction equation. The transport equations for continuity, momentum, energy, and turbulence were transformed into their finite-volume algorithms by integrating over the computational cells of the active domain. The set of simultaneous algebraic equations was solved using a line-by-line semi-implicit iterative scheme that is directionally altered in the three-dimensional structure. The simulation, including the turbulence k-ε model, DO radiation model, and melting/vaporization control code was incremented in one-minute time steps until no liquid agent remained in the ton container. The energy equation used in the model algorithm was modified by the melting/vaporization code in each time step. This created a powerful model that can be used to simulate the vaporization of any liquid, solid, or liquid with solid agent mass within the ton container.

CFD Model Calibration

The PVR and CFD models were calibrated using TOCDF ton container processing data from March 13, 2004 for 45 pounds mass (lbm) of VX heel. Summaries of key process parameters from this data are shown in Table 8 and Figure 5. Table 8 gives an estimate of agent vaporization based on furnace temperature and water spray flow for ten ton containers. The average vaporization starting time is 21 minutes. The average peak vaporization rate occurred at 39.5 minutes. Figure 5 shows key process conditions during processing of tray number 10. Using the data presented in Figure 5, it was estimated that vaporization started 20 minutes after the container was fed to the furnace and the peak vaporization rate occurred at 39.5 minutes following container feed. It is difficult to define the vaporization end time based on furnace and crossover duct temperatures because of the refractory thermal inertia.

The agent vaporization rates predicted by CR&E's PVR and CFD models for processing of a ton container with a 45 lbm VX heel are compared to the TOCDF process data in Table 9. The vaporization start time predicted by the PVR model is 20 minutes. The CFD model predicts a vaporization start time of 23 minutes. Peak vaporization occurs at 32 minutes for the PVR model and 35 minutes for the CFD model. The agent vaporization start and peak times predicted by the PVR and CFD models are in good agreement with the TOCDF 45 lbm VX ton container process data.

Table 8: TOCDF 45 lbm VX Ton Container Agent Vaporization Predictions from Processing Data of March 13, 2004

Tray No.	Vap. Start Time (min)	Peak Vaporization time (min)
2	22:30	37:30
3	21:00	40:30
4	19:00	40:00
5	19:30	37:30
6	18:30	41:00
7	24:00	34:30
8	19:00	40:00
9	22:30	43:30
10	20:00	39:30
11	23:30	41:00
Average	21:00	39.30

Table 9: PVR and CFD Model Predicted Results with TOCDF Ton Container Processing Data on March 18, 2004 for 45 lbm VX Heel

	Vap. Start Time (min)	PVR time (min)	Vap. End Time (min)
TOCDF data	21:00	39:30	
PVR model	20:00	32:00	43:00
CFD model	23:00	35:00	41:00

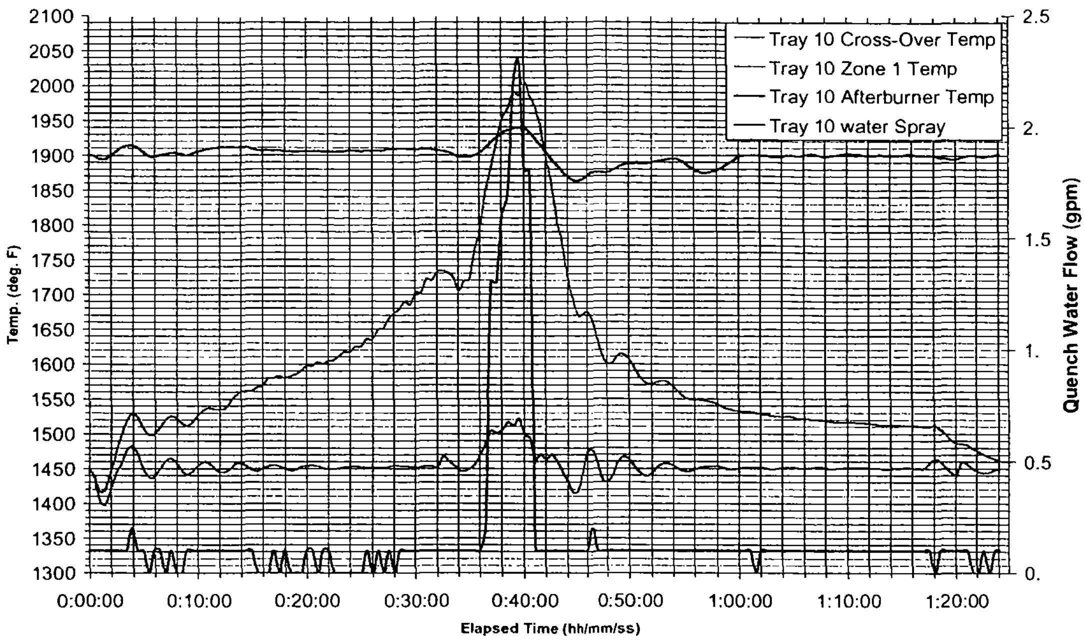


Figure 5: March 13, 2004 TOCDF VX Ton Container Key Process Data for Tray 10 having a 45 lbm Heel

Model Results – Simulation 1 (MPF @ 1,450°F)

The calibrated CFD model was used to predict agent vaporization from seven ton container cases. Each case modeled was defined with a different center HD solid heel depth and solid heel end profile. All cases contained 2 inches of liquid HD over the solid heel as shown in Figure 4. The CFD model calculates heat and mass transfer to the agent to simulate the melting and vaporization processes. The solid portion of the heel begins to melt when it reaches a temperature of 212°F. The solid agent melts and merges with the liquid HD to form a single liquid agent pool. The liquid agent continues to be heated until it reaches a vaporization temperature of 463.73°F. The agent begins to vaporize as it continues to be heated. The latent heat of HD solid heel melting and liquid HD vaporization is 87.075 Btu/lbm and 285.52 Btu/lbm, respectively.

The HD liquid properties used in the CFD model are the same as those used in the CR&E PVR model shown in Table 4. The HD solid heel properties are listed in Table 5. Two scalars in the vaporization control code are used to measure the solid mass fraction and liquid mass fraction. The predicted agent vaporization rate for each of the seven cases are shown in Figures 6-12 and summarized in Table 10. Calculated vaporization data is presented in Appendix A. The curve shown as a solid line in Figures 6-12 is a plot of the CFD generated vaporization data. The curve shown as a dashed line is a sixth order polynomial trended curve based on the CFD generated vaporization data. Table 10 is provided as a comparison of the results for all seven cases modeled.

Figure 6 shows the HD vaporization rate curve for a 1 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 31.64 lbm. The liquid heel mass is 87.15 lbm. The total heel mass is 118.79 lbm. The agent begins to vaporize after a furnace time of 33 minutes. The predicted peak vaporization rate is 305.97 lbm/hr occurring at 49 minutes. The predicted duration of agent vaporization is 68 minutes.

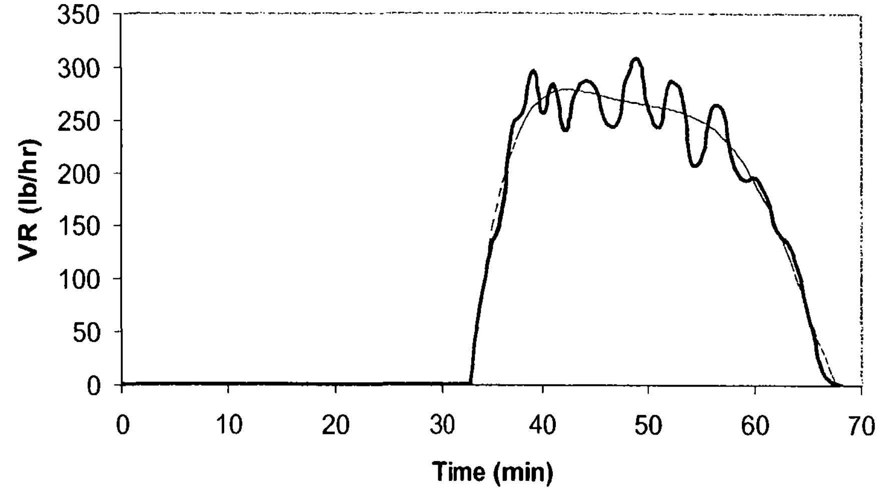


Figure 6: Vaporization rate curve for 1 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,450°F

Figure 7 shows the HD vaporization rate curve for a 2 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 100.11 lbm. The liquid heel mass is 96.47 lbm. The total heel mass is 196.58 lbm. The agent begins to vaporize after a furnace time of 37 minutes. The predicted peak vaporization rate is 359.25 lbm/hr and occurs at 51 minutes. The predicted duration of agent vaporization is 85 minutes.

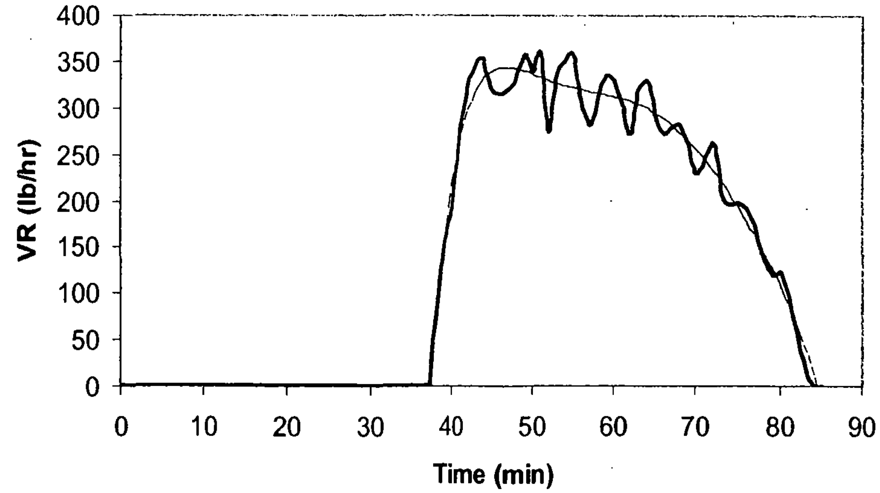


Figure 7: Vaporization rate curve for 2 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,450°F

Figure 8 shows the HD vaporization rate curve for a 3 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 201.77 lbm. The liquid heel mass is 102.11 lbm. The total heel mass is 303.88 lbm. The agent begins to vaporize after a furnace time of 40 minutes. The predicted peak vaporization rate is 450.33 lbm/hr and occurs at 54 minutes. The predicted duration of agent vaporization is 106 minutes.

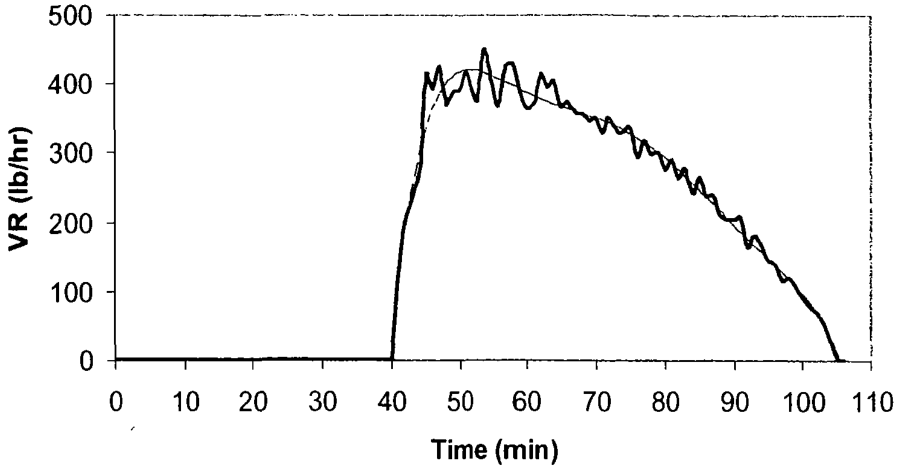


Figure 8: Vaporization rate curve for 3 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,450°F

Figure 9 shows the HD vaporization rate curve for a 4 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 335.41 lbm. The liquid heel mass is 103.9 lbm. The total heel mass is 439.31 lbm. The agent begins to vaporize after a furnace time of 45 minutes. The predicted peak vaporization rate is 501.94 lbm/hr and occurs at 59 minutes. The predicted duration of agent vaporization is 130 minutes.

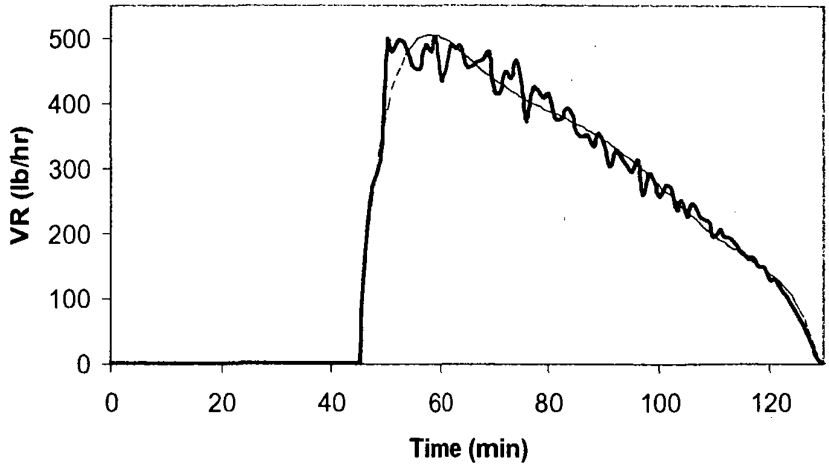


Figure 9: Vaporization rate curve for 4 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,450°F

Figure 10 shows the HD vaporization rate curve for a 5 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 422.13 lbm. The liquid heel mass is 111.55 lbm. The total heel mass is 533.68 lbm. The agent begins to vaporize after a furnace time of 47 minutes. The predicted peak vaporization rate is 554.1 lbm/hr and occurs at 64 minutes. The predicted duration of agent vaporization is 145 minutes.

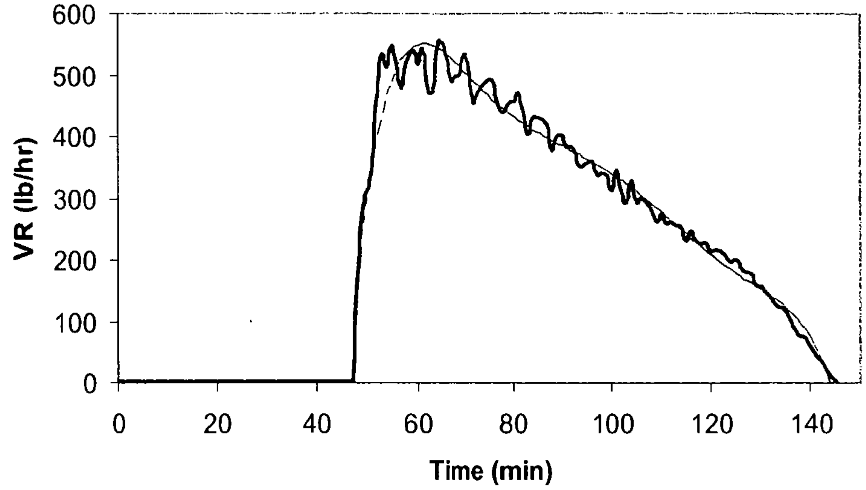


Figure 10: Vaporization rate curve for 5 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,450°F

Figure 11 shows the HD vaporization rate curve for a 6 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 514.55 lbm. The liquid heel mass is 117.96 lbm. The total heel mass is 632.51 lbm. The agent begins to vaporize after a furnace time of 51 minutes. The predicted peak vaporization rate is 598.2 lbm/hr and occurs at 68 minutes. The predicted duration of agent vaporization is 163 minutes.

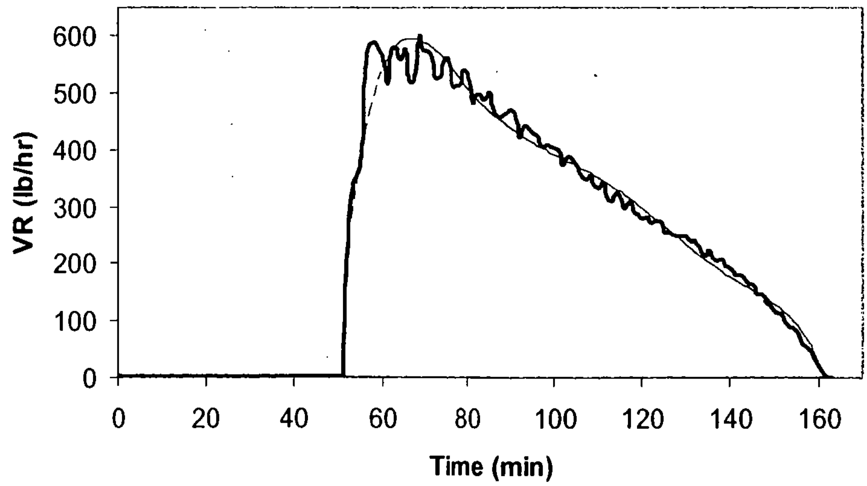


Figure 11: Vaporization rate curve for 6 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,450°F

Figure 12 shows the HD vaporization rate curve for a 7 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 611.71 lbm. The liquid heel mass is 123.32 lbm. The total heel mass is 735.03 lbm. The agent begins to vaporize after a furnace time of 56 minutes. The predicted peak vaporization rate is 649.04 lbm/hr and occurs at 74 minutes. The predicted duration of agent vaporization is 180 minutes.

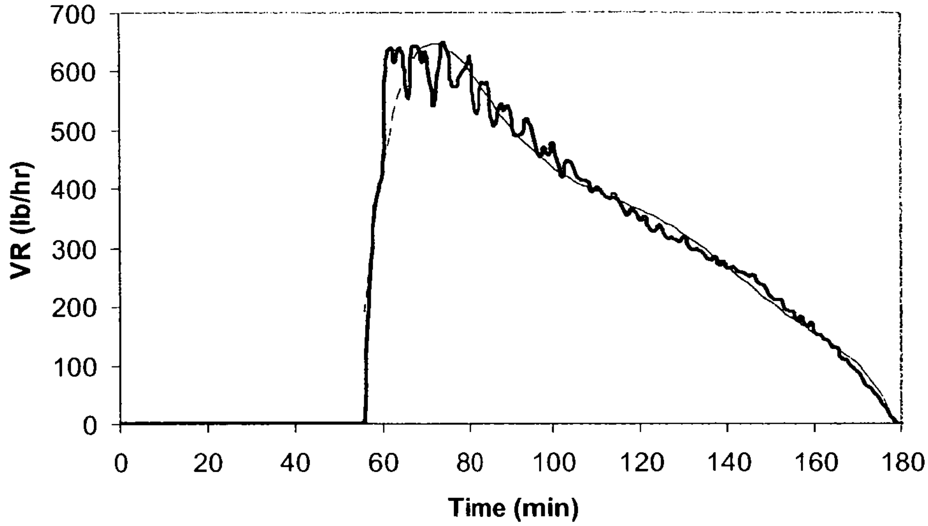


Figure 12: Vaporization rate curve for 7 inch HD solid heel and 2 inches of liquid HD at and MPF operating at 1,450°F

Table10: Ton Container CFD Model Predicted Vaporization Rates and Times for Varying Heels and MPF Operating at 1,450°F

Case	Total HD Mass (lbm)	Vap. Start Time (min)	PVR (lbm/hr)	PVR Time (min)	Vap. End Time (min)
1" solid with 2" top liquid HD	118.79	33	305.97	49	68
2" solid with 2" top liquid HD	196.58	37	359.25	51	85
3" solid with 2" top liquid HD	303.88	40	450.33	54	106
4" solid with 2" top liquid HD	439.31	45	501.94	59	130
5" solid with 2" top liquid HD	533.68	47	554.1	64	145
6" solid with 2" top liquid HD	632.51	51	598.2	68	163
7" solid with 2" top liquid HD	735.03	56	649.04	74	180

Processing Evaluation and Optimization

The CFD model predicted vaporization rates and times for varying heels were entered into the CR&E Mass and Energy balance model in order to evaluate furnace performance and optimize the ton container processing rate. Mass and energy balance calculations were completed for all of the CFD model cases. Furnace operating conditions were examined for each case to determine if there were any conditions that would limit processing. Key conditions examined were furnace primary temperature, maximum quench water flow, minimum primary exit gas oxygen, afterburner fume air required, exit gas temperature, minimum afterburner gas residence time, and minimum exit gas oxygen.

Furnace throughput rate was optimized for each case by varying the tray feed interval within the constraints of 5X requirements and furnace capabilities. A tray feed interval that is less than the time required for complete agent vaporization will result in agent vaporization in both Zones 1 and Zone 2 (a tray will progress from Zone 1 into Zone 2 while continuing to vaporize as a new tray is loaded into Zone 1). This results in a total agent vaporization rate within the furnace which is the sum of the vaporization rates of each tray at each time step. The minimum feed interval between the trays was determined by the shortest feed time (maximum tray vaporization overlap) which would not result in a total vaporization rate in excess of the peak vaporization rate of a single tray.

Figure 13 shows an example of the overlap of agent vaporization that occurs during optimized tray feed cycles. Other constraints utilized in determination of the optimum tray feed interval were that the tray remain in the furnace long enough to meet the "5X" criteria and no vaporization is allowed to occur in Zone 3. Table 11 gives a summary of optimum processing conditions determined for ton containers with the investigated solid heel depths and 2 inches of liquid agent over the top of the solid.

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Table 11: TOCDF HD Ton Container Processing Summary (MPF Operating at 1,450°F)

MUNITION & FURNACE RUN PROPERTIES								
Agent/Heel:	HD 1" Solid + 2" Liquid Heel	HD 2" Solid + 2" Liquid Heel	HD 3" Solid + 2" Liquid Heel	HD 4" Solid + 2" Liquid Heel	HD 5" Solid + 2" Liquid Heel	HD 6" Solid + 2" Liquid Heel	HD 7" Solid + 2" Liquid Heel	
Munition:	Ton Container	Ton Container	Ton Container	Ton Container	Ton Container	Ton Container	Ton Container	
Tray Feed Interval:	31	41	59	79	91	104	116	minutes
5X MIN Residence:	84	102	122	146	162	180	196	minutes
Throughput:	1.94	1.46	1.02	0.76	0.66	0.58	0.52	TC/Hr
PRIMARY								
Fuel MIN SP:	350	350	350	350	350	350	350	scfh per burner
Comb. Air per Burner:	255	255	255	255	255	255	255	scfm
Zone 2 burners:	3	3	3	3	3	3	3	of 4
Exit Gas Temp. Set Point:	1450	1450	1450	1450	1450	1450	1450	°F
MPF Quench Nozzles								
MAX Quench (Req'd):	0	0	0	0	46	221	424	lbm/Hr
MAX Quench (Req'd):	0.0	0.0	0.0	0.0	0.1	0.4	0.8	gpm [6 nozzles]
Flue Gas Oxygen MIN:	15.32%	15.29%	15.25%	15.23%	15.11%	14.71%	14.26%	% [Limit 3.0%]
AFTERBURNER								
CA: FG Ratio:	12.0	12.0	12.0	12.0	12.0	12.0	12.0	to 1
Fume Air flow SP:	300	300	300	300	300	300	300	scfm
Fume Air flow @ MAX Vap.:	0	0	0	0	0	0	0	scfm
Exit Gas Temp. Set Point:	2000	2000	2000	2000	2000	2000	2000	°F
AFB MIN Residence:	1.30	1.30	1.30	1.30	1.29	1.26	1.23	sec [1.0 sec MIN]
Flue Gas Oxygen MIN:	12.15%	12.14%	12.12%	12.11%	12.01%	11.67%	11.29%	% [Limit 3.0%]
Exit Flue Gas Flow:	19,667	19,701	19,760	19,793	19,916	20,286	20,712	lbm/Hr

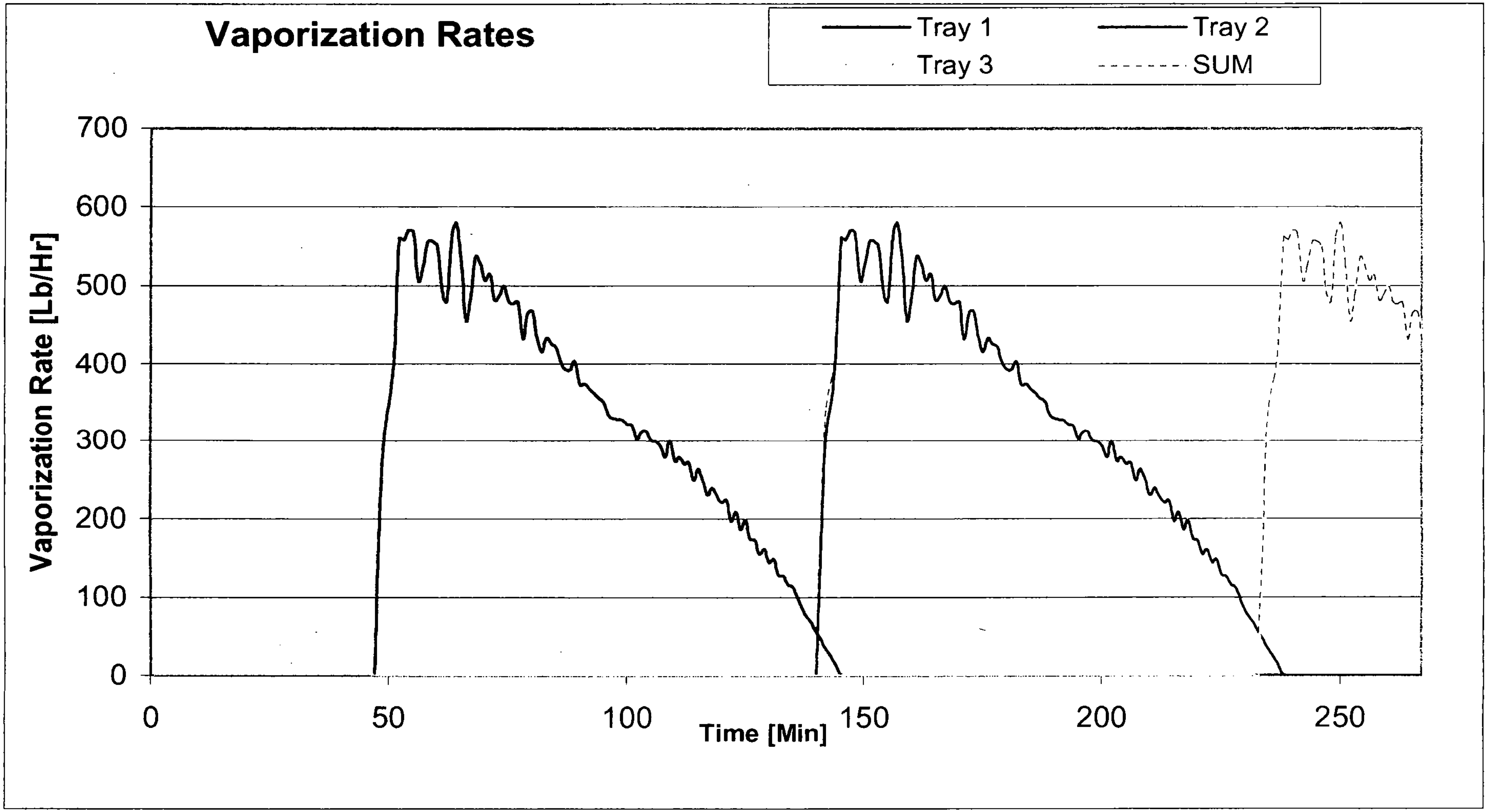

Figure 13: TOCDF HD Ton Container Processing Optimization (MPF Operating at 1,450°F)

Model Results – Simulation 2 (MPF @ 1,600°F)

The predicted agent vaporization rate for each of the seven cases are shown in Figures 14-20 and summarized in Table 12. Calculated vaporization data is presented in Appendix B. The curve shown as a solid line in Figures 14-20 is a plot of the CFD generated vaporization data. The curve shown as a dashed line is a sixth order polynomial trended curve based on the CFD generated vaporization data. Table 12 is provided as a comparison of the results for all seven cases modeled.

Figure 14 shows the HD vaporization rate curve for a 1 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 31.64 lbm. The liquid heel mass is 87.15 lbm. The total heel mass is 118.79 lbm. The agent begins to vaporize after a furnace time of 27 minutes. The predicted peak vaporization rate is 354.4 lbm/hr occurring at 32 minutes. The predicted duration of agent vaporization is 56 minutes.

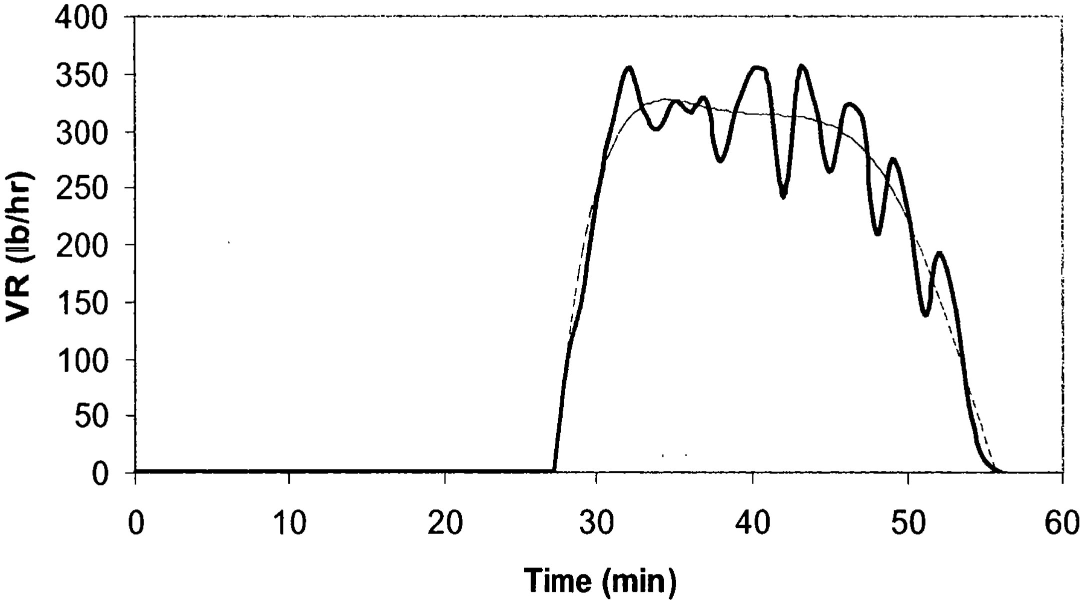

Figure 14: Vaporization rate curve for 1 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,600°F

Figure 15 shows the HD vaporization rate curve for a 2 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 100.11 lbm. The liquid heel mass is 96.47 lbm. The total heel mass is 196.58 lbm. The agent begins to vaporize after a furnace time of 29 minutes. The predicted peak vaporization rate is 435.57 lbm/hr and occurs at 35 minutes. The predicted duration of agent vaporization is 70 minutes.

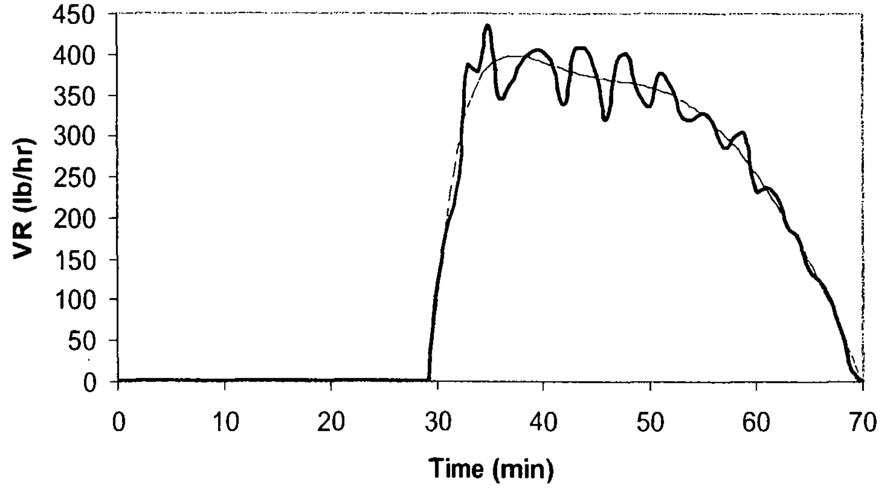

Figure 15: Vaporization rate curve for 2 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,600°F

Figure 16 shows the HD vaporization rate curve for a 3 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 201.77 lbm. The liquid heel mass is 102.11 lbm. The total heel mass is 303.88 lbm. The agent begins to vaporize after a furnace time of 32 minutes. The predicted peak vaporization rate is 513.78 lbm/hr and occurs at 42 minutes. The predicted duration of agent vaporization is 89 minutes.

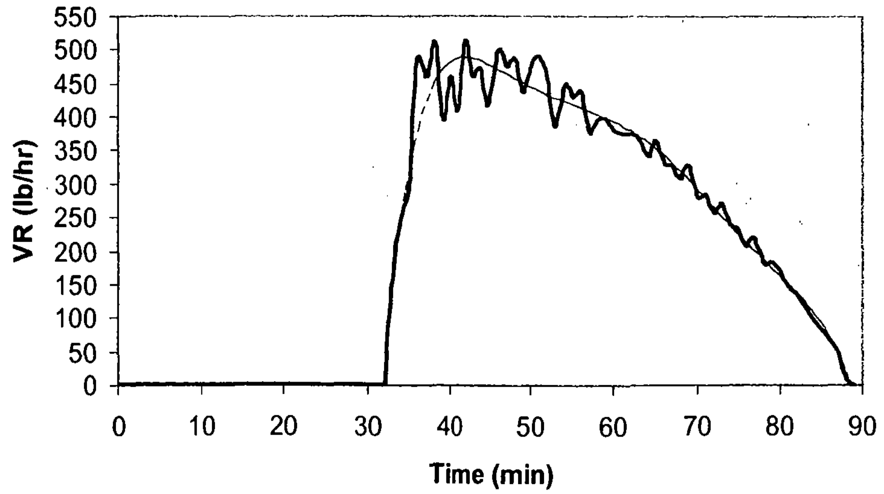

Figure 16: Vaporization rate curve for 3 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,600°F

Figure 17 shows the HD vaporization rate curve for a 4 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 335.41 lbm. The liquid heel mass is 103.9 lbm. The total heel mass is 439.31 lbm. The agent begins to vaporize after a furnace time of 34 minutes. The predicted peak vaporization rate is 589.26 lbm/hr and occurs at 46 minutes. The predicted duration of agent vaporization is 106 minutes.

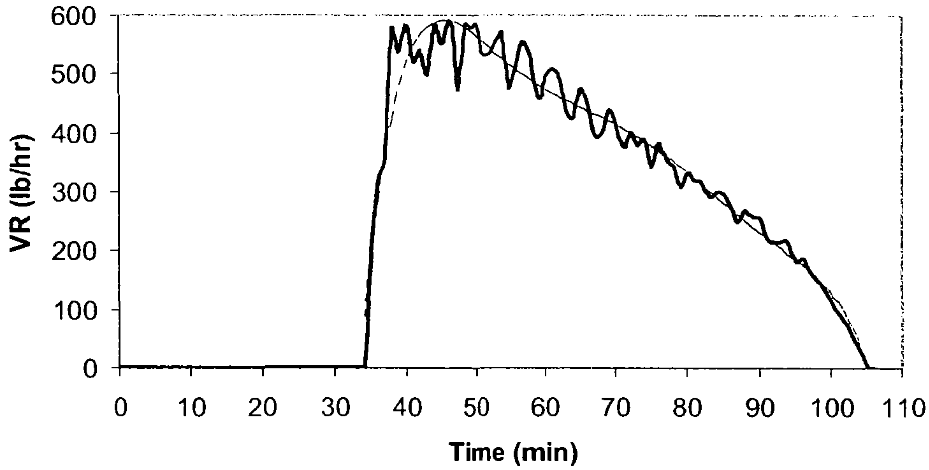

Figure 17: Vaporization rate curve for 4 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,600°F

Figure 18 shows the HD vaporization rate curve for a 5 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 422.13 lbm. The liquid heel mass is 111.55 lbm. The total heel mass is 533.68 lbm. The agent begins to vaporize after a furnace time of 37 minutes. The predicted peak vaporization rate is 653.5 lbm/hr and occurs at 52 minutes. The predicted duration of agent vaporization is 120 minutes.

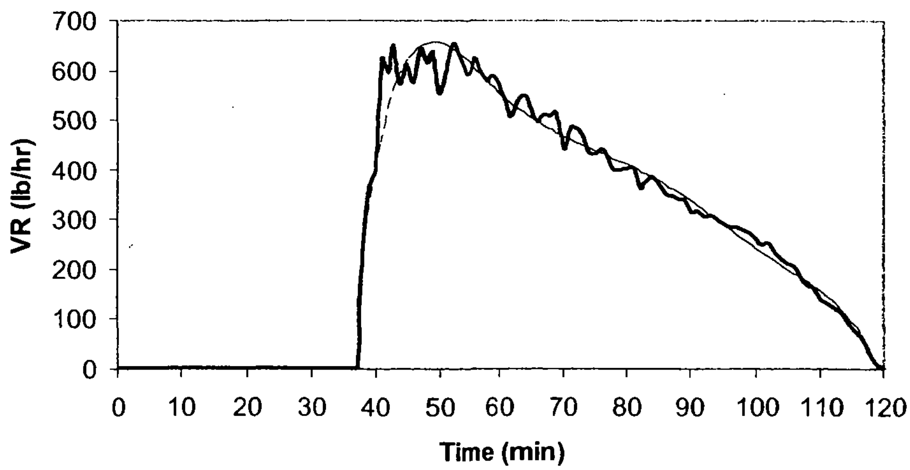

Figure 18: Vaporization rate curve for 5 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,600°F

Figure 19 shows the HD vaporization rate curve for a 6 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 514.55 lbm. The liquid heel mass is 117.96 lbm. The total heel mass is 632.51 lbm. The agent begins to vaporize after a furnace time of 40 minutes. The predicted peak vaporization rate is 724.44 lbm/hr and occurs at 55 minutes. The predicted duration of agent vaporization is 135 minutes.

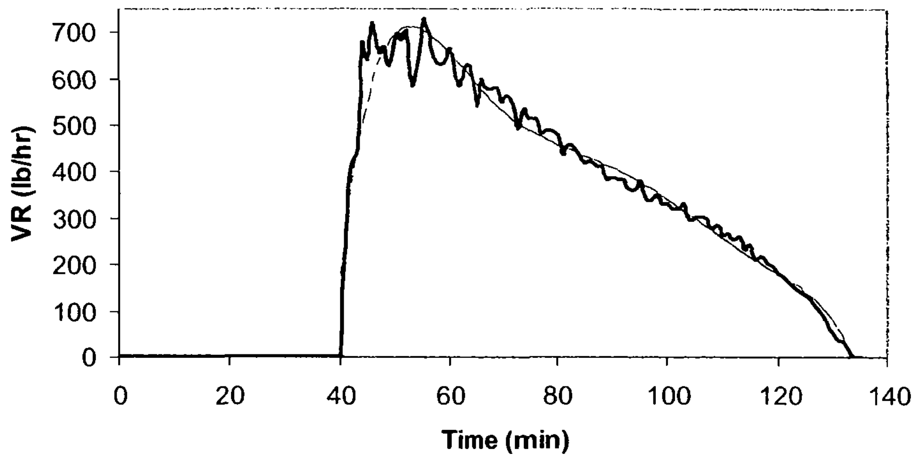

Figure 19: Vaporization rate curve for 6 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1,600°F

Figure 20 shows the HD vaporization rate curve for a 7 inch HD solid heel and 2 inches of liquid HD. The solid heel mass is 611.71 lbm. The liquid heel mass is 123.32 lbm. The total heel mass is 735.03 lbm. The agent begins to vaporize after a furnace time of 44 minutes. The predicted peak vaporization rate is 793.62 lbm/hr and occurs at 59 minutes. The predicted duration of agent vaporization is 148 minutes.

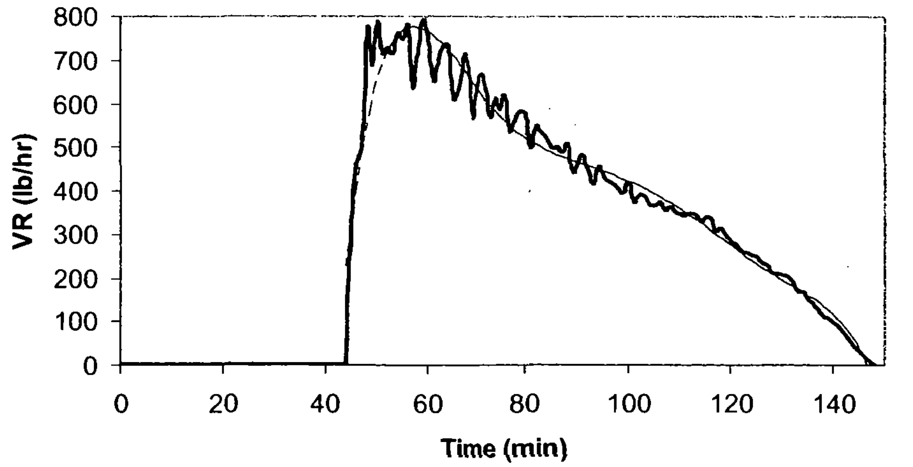

Figure 20: Vaporization rate curve for 7 inch HD solid heel and 2 inches of liquid HD and MPF operating at 1600°F

Table 12: Ton Container CFD Model Predicted Vaporization Rates and Times for Varying Heels and MPF Operating at 1,600°F

Case	Total HD Mass (lbm)	Vap. Start Time (min)	PVR (lbm/hr)	PVR Time (min)	Vap. End Time (min)
1" solid with 2" top liquid HD	118.79	27	354.4	32	56
2" solid with 2" top liquid HD	196.58	29	435.57	35	70
3" solid with 2" top liquid HD	303.88	32	513.78	42	89
4" solid with 2" top liquid HD	439.31	34	589.26	46	106
5" solid with 2" top liquid HD	533.68	37	653.5	52	120
6" solid with 2" top liquid HD	632.51	40	724.44	55	135
7" solid with 2" top liquid HD	735.03	44	793.62	59	148

Processing Evaluation and Optimization – Simulation 2 (MPF @ 1,600°F)

The CFD model predicted vaporization rates and times for varying heels were entered into the CR&E Mass and Energy balance model in order to evaluate furnace performance and optimize the ton container processing rate. Mass and Energy balance calculations were completed for all of the CFD model cases. Furnace operating conditions were examined for each case to determine if there were any conditions that would limit processing. Key conditions examined were furnace primary temperature, maximum quench water flow, minimum primary exit gas oxygen, afterburner fume air required, exit gas temperature, minimum afterburner gas residence time, and minimum exit gas oxygen.

Furnace throughput rate was optimized for each case by varying the tray feed interval within the constraints of 5X requirements and furnace capabilities. A tray feed interval that is less than the time required for complete agent vaporization will result in agent vaporization in both Zones 1 and Zone 2 (a tray will progress from Zone 1 into Zone 2 while continuing to vaporize as a new tray is loaded into Zone 1). This results in a total agent vaporization rate within the furnace which is the sum of the vaporization rates of each tray at each time step. The minimum feed interval between the trays was determined by the shortest feed time (maximum tray vaporization overlap) which would not result in a total vaporization rate in excess of the peak vaporization rate of a single tray.

Figure 21 shows an example of the overlap of agent vaporization that occurs during optimized tray feed cycles. Other constraints utilized in determination of the optimum tray feed interval were that the tray remain in the furnace long enough to meet the "5X" criteria and no vaporization is allowed to occur in zone 3. Table 13 gives a summary of optimum processing conditions determined for ton containers with the investigated solid heel depths and 2 inches of liquid agent over the top of the solid.

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Table 13: TOCDF HD Ton Container Processing Summary (MPF Operating at 1,600°F)

MUNITION & FURNACE RUN PROPERTIES								
Agent/Heel:	HD 1" Solid + 2" Liquid Heel	HD 2" Solid + 2" Liquid Heel	HD 3" Solid + 2" Liquid Heel	HD 4" Solid + 2" Liquid Heel	HD 5" Solid + 2" Liquid Heel	HD 6" Solid + 2" Liquid Heel	HD 7" Solid + 2" Liquid Heel	
Munition:	Ton Container	Ton Container	Ton Container	Ton Container	Ton Container	Ton Container	Ton Container	
Tray Feed Interval:	24	36	52	67	77	88	98	minutes
5X MIN Residence:	72	86	106	122	136	152	164	minutes
Throughput:	2.5	1.67	1.15	0.9	0.78	0.68	0.61	TC/Hr
PRIMARY								
Fuel MIN SP:	350	350	350	350	350	350	350	scfh per burner
Comb. Air per Burner:	255	255	255	255	255	255	255	scfm
Zone 2 burners:	3	3	3	3	3	3	3	of 4
Exit Gas Temp. Set Point:	1600	1600	1600	1600	1600	1600	1600	°F
MPF Quench Nozzles								
MAX Quench (Req'd):	0	0	0	0	99	366	627	lbm/Hr
MAX Quench (Req'd):	0.0	0.0	0.0	0.0	0.2	0.7	1.3	gpm [6 nozzles]
Flue Gas Oxygen MIN:	14.56%	14.53%	14.5%	14.47%	14.22%	13.58%	12.97%	% [Limit 3.0%]
AFTERBURNER								
CA: FG Ratio:	12.0	12.0	12.0	12.0	12.0	12.0	12.0	to 1
Fume Air flow SP:	300	300	300	300	300	300	300	scfm
Fume Air AVG flow:	0	0	0	0	0	0	0	scfm
Exit Gas Temp. Set Point:	2000	2000	2000	2000	2000	2000	2000	°F
AFB MIN Residence:	1.39	1.39	1.39	1.39	1.37	1.33	1.29	sec [1.0 sec MIN]
Flue Gas Oxygen MIN:	12.12%	12.1%	12.08%	12.07%	11.85%	11.3%	10.78%	% [Limit 3.0%]
Exit Flue Gas Flow:	18,412	18,464	18,514	18,563	18,776	19,283	19,778	lbm/Hr

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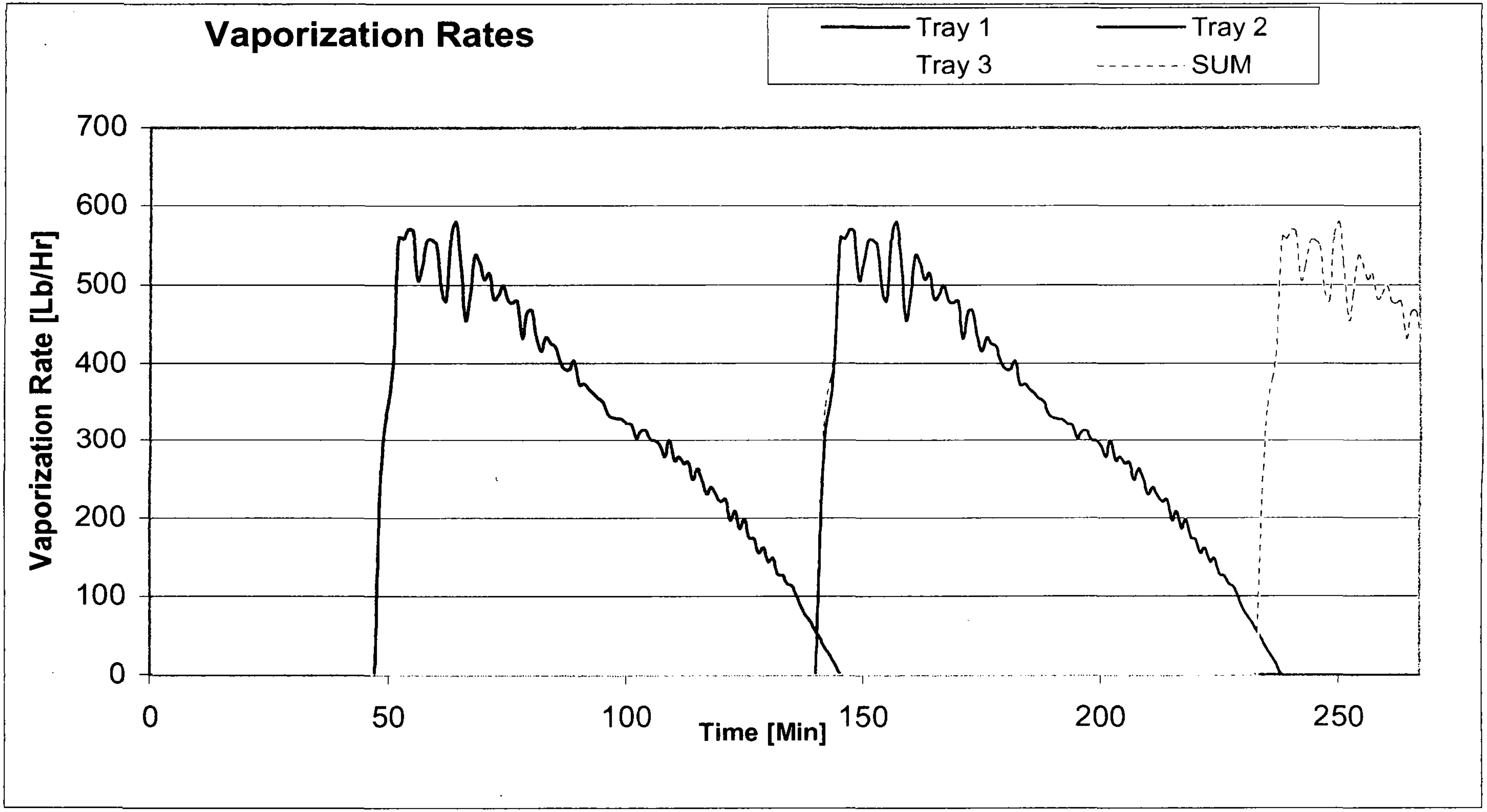

Figure 21: TOCDF HD Ton Container Processing Optimization (MPF Operating at 1,600°F)

Model Results – Comparison of Operating Temperature Results

Increasing the MPF operating temperature will reduce the time required to changeover from processing ton containers to secondary waste or other wastes. The predicted vaporization rate for each of the seven cases is provided in Figures 21-27. The red curve represents the vaporization rate at an operating temperature of 1,600°F, and the blue curve represents the vaporization rate at an operating temperature of 1,450°F.

Figure 21 shows the vaporization rate comparison for a 1 inch HD solid heel and 2 inches of liquid HD case at furnace operating temperatures of 1,600°F and 1,450°F. Increasing the operating temperature from 1,450°F to 1,600°F results in the vaporization start time reducing from 33 minutes to 27 minutes, peak vaporization rate increasing from 305.97 to 354.4 lbm/hr, peak vaporization time reducing from 49 minutes to 32 minutes, and vaporization end time reducing from 68 minutes to 56 minutes.

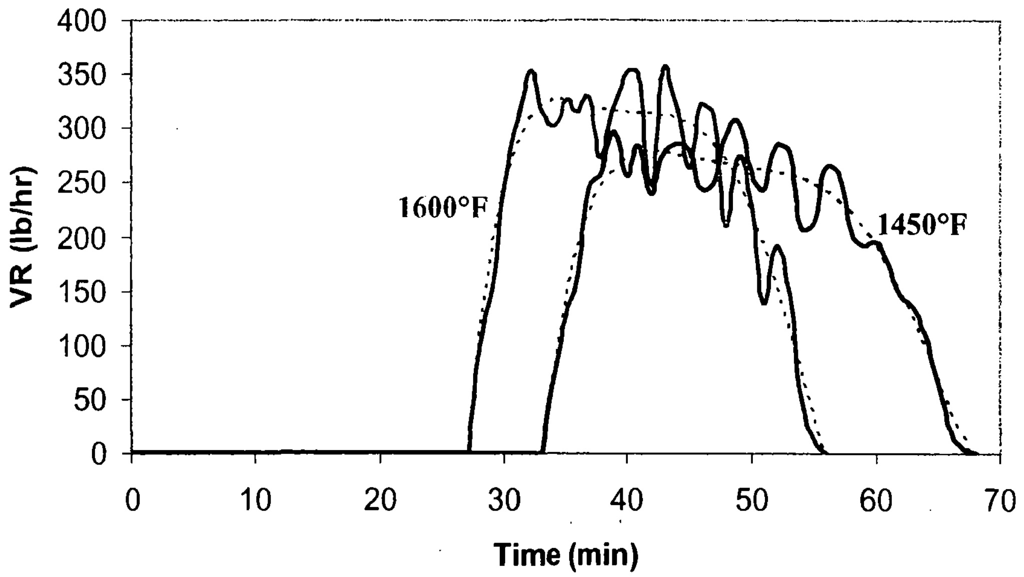

Figure 21: Vaporization rate curve for 1 inch HD solid heel case
with MPF operating at 1,450°F and 1,600°F

Figure 22 shows the vaporization rate comparison for a 2 inch HD solid heel and 2 inches of liquid HD case at furnace operating temperatures of 1,600°F and 1,450°F. Increasing the operating temperature from 1,450°F to 1,600°F results in the vaporization start time reducing from 37 minutes to 29 minutes, peak vaporization rate increasing from 359.25 to 435.57 lbm/hr, peak vaporization time reducing from 51 minutes to 35 minutes, and vaporization end time reducing from 85 minutes to 70 minutes.

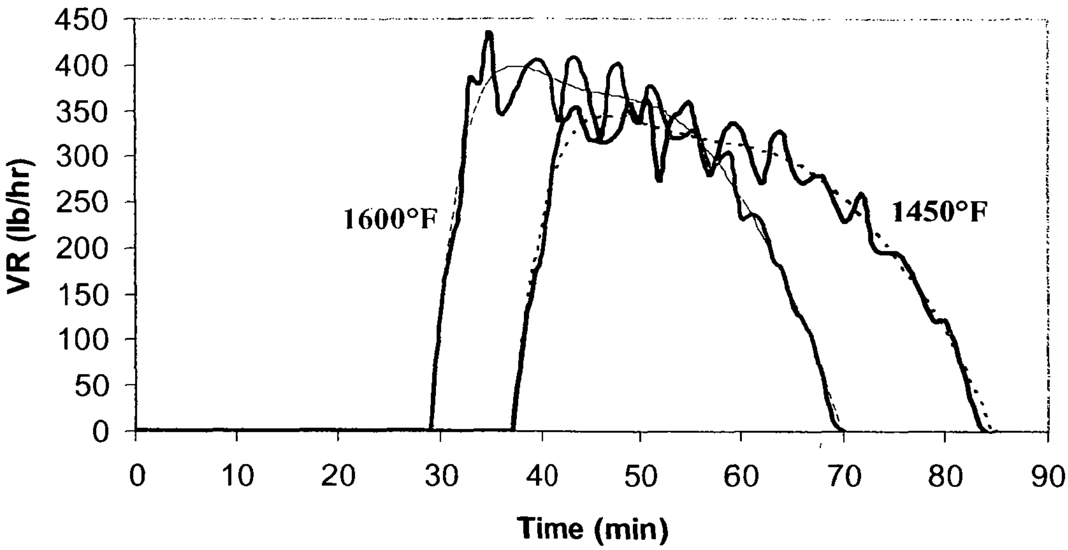

Figure 22: Vaporization rate curve for 2 inch HD solid heel case with MPF operating at 1,450°F and 1,600°F

Figure 23 shows the vaporization rate comparison for a 3 inch HD solid heel and 2 inches of liquid HD case at furnace operating temperatures of 1,600°F and 1,450°F. Increasing the operating temperature from 1,450°F to 1,600°F results in the vaporization start time reducing from 40 minutes to 32 minutes, peak vaporization rate increasing from 450.33 to 513.78 lbm/hr, peak vaporization time reducing from 54 minutes to 42 minutes, and vaporization end time reducing from 106 minutes to 89 minutes.

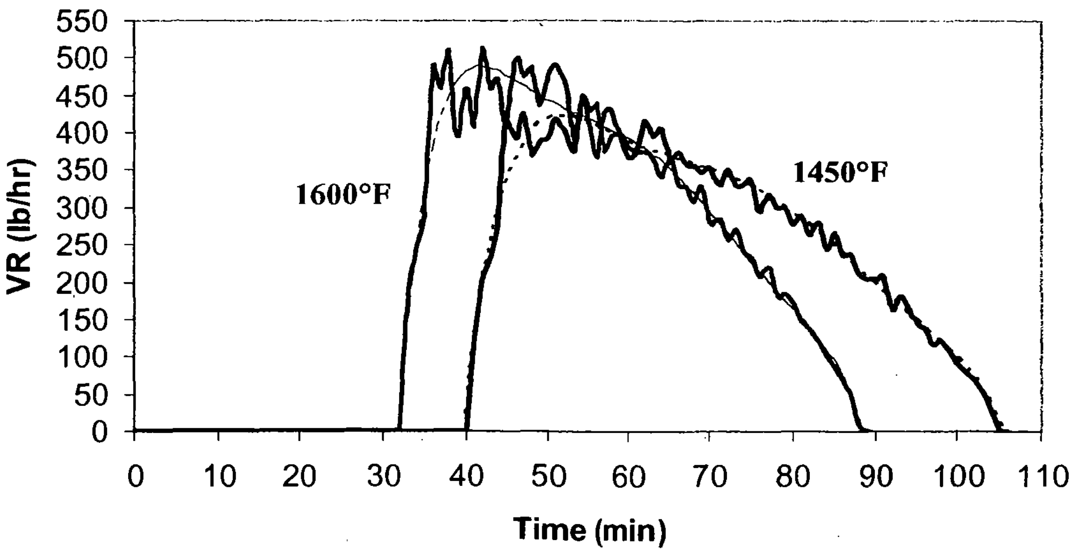

Figure 23: Vaporization rate curve for 3 inch HD solid heel case with MPF operating at 1,450°F and 1,600°F

Figure 24 shows the vaporization rate comparison for a 4 inch HD solid heel and 2 inches of liquid HD case at furnace operating temperatures of 1,600°F and 1,450°F. Increasing the operating temperature from 1,450°F to 1,600°F results in the vaporization start time reducing from 45 minutes to 34 minutes, peak vaporization rate increasing from 501.94 to 589.26 lbm/hr, peak vaporization time reducing from 59 minutes to 46 minutes, and vaporization end time reducing from 130 minutes to 106 minutes.

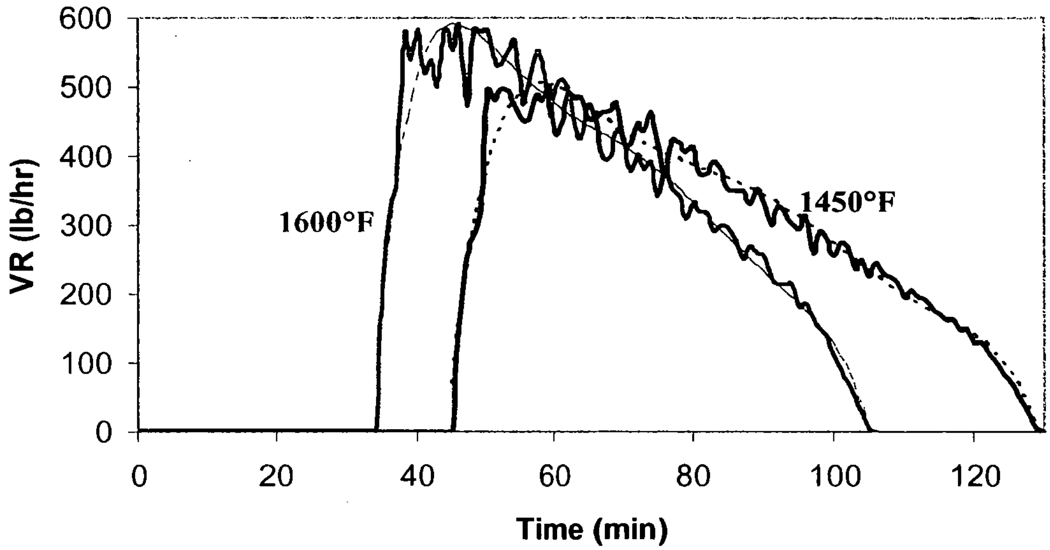

Figure 24: Vaporization rate curve for 4 inch HD solid heel case with MPF operating at 1,450°F and 1,600°F

Figure 25 shows the vaporization rate comparison for a 5 inch HD solid heel and 2 inches of liquid HD case at furnace operating temperatures of 1,600°F and 1,450°F. Increasing the operating temperature from 1,450°F to 1,600°F results in the vaporization start time reducing from 47 minutes to 37 minutes, peak vaporization rate increasing from 554.1 to 653.5 lbm/hr, peak vaporization time reducing from 64 minutes to 52 minutes, and vaporization end time reducing from 145 minutes to 120 minutes.

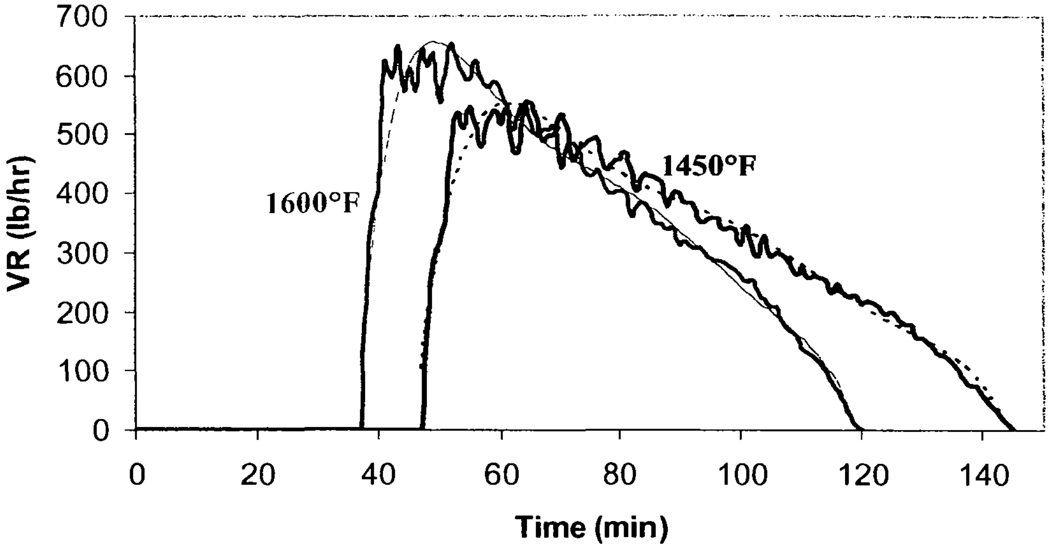

Figure 25: Vaporization rate curve for 5 inch HD solid heel case with MPF operating at 1,450°F and 1,600°F

Figure 26 shows the vaporization rate comparison for a 6 inch HD solid heel and 2 inches of liquid HD case at furnace operating temperatures of 1,600°F and 1,450°F. Increasing the operating temperature from 1,450°F to 1,600°F results in the vaporization start time reducing from 51 minutes to 40 minutes, peak vaporization rate increasing from 598.2 to 724.44 lbm/hr, peak vaporization time reducing from 68 minutes to 55 minutes, and vaporization end time reducing from 163 minutes to 135 minutes.

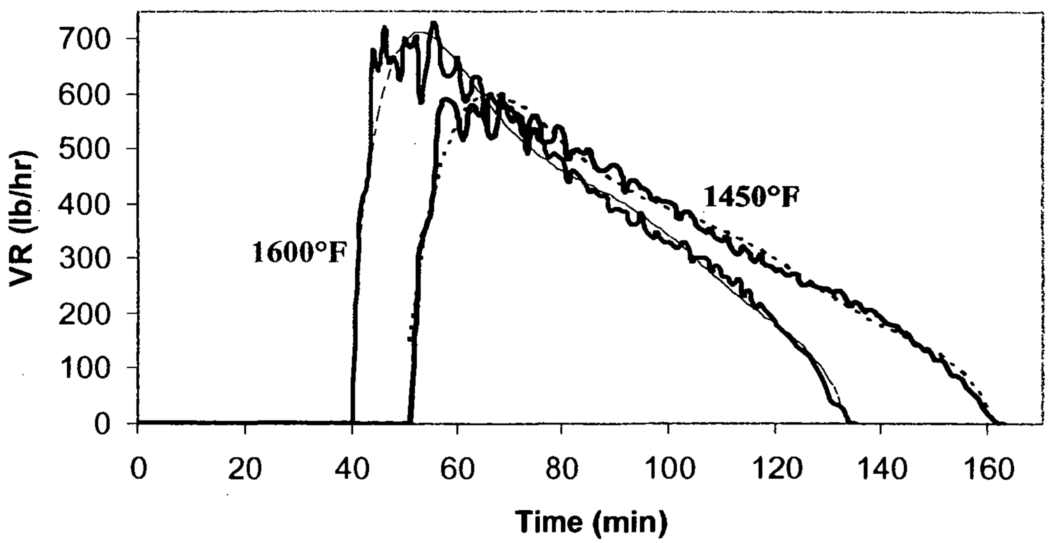

Figure 26: Vaporization rate curve for 6 inch HD solid heel case with MPF operating at 1,450°F and 1,600°F

Figure 27 shows the vaporization rate comparison for a 7 inch HD solid heel and 2 inches of liquid HD case at furnace operating temperatures of 1,600°F and 1,450°F. Increasing the operating temperature from 1,450°F to 1,600°F results in the vaporization start time reducing from 56 minutes to 44 minutes, peak vaporization rate increasing from 649.04 to 793.62 lbm/hr, peak vaporization time reducing from 74 minutes to 59 minutes, and vaporization end time reducing from 180 minutes to 148 minutes.

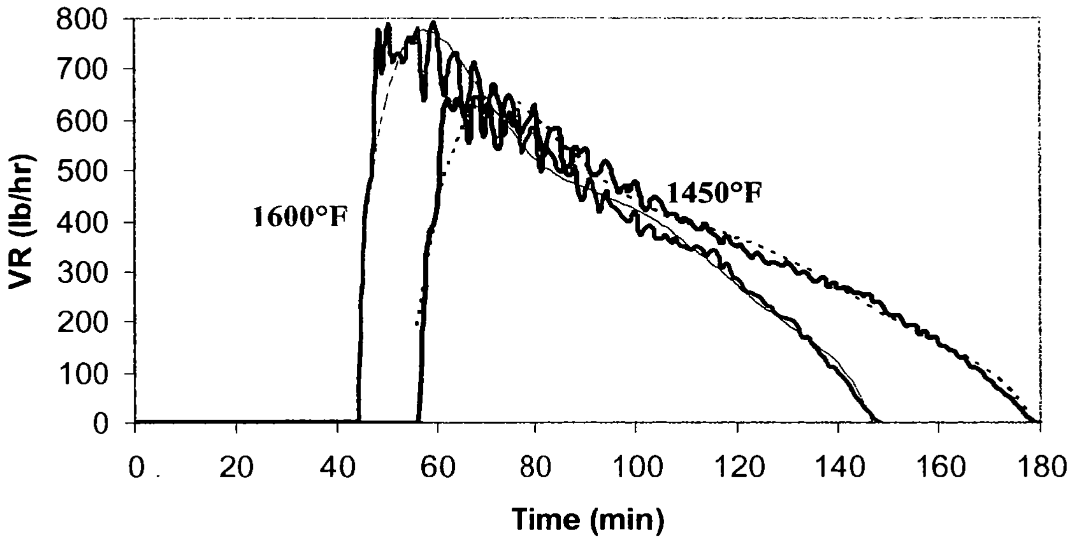

Figure 27: Vaporization rate curve for 7 inch HD solid heel case with MPF operating at 1,450°F and 1,600°F

Other Processing Considerations

The water spray nozzle orientation may be a limitation to the efficient processing of HD on containers with various solid heel depths. The nozzles at TOCDF are located on the side of the furnace and spray horizontally over the top of the tray. This spray orientation directs the water over the top of the munitions load and toward the opposite side of the furnace. The furnace temperature control thermocouples are located at the top of the furnace chamber. The horizontal water spray pattern is likely to cause inaccurate temperature readings from these thermocouples due to water spray impingement. The purpose of water sprays in Zones 1 and 2 are for control of furnace temperature during peak agent vaporization. Water sprays directed vertically downward toward the munitions being processed most efficiently accomplishes this. It is recommended that consideration be given to relocating the water spray nozzles to a vertical downward orientation in order to aid in furnace temperature control during processing of the HD ton containers.

The potential for processed ton containers containing HD to exhibit smoking when exiting the discharge airlock was evaluated. Agent HD has a molecular formula of $C_4H_8Cl_2S$, and is classified as a halogenated hydrocarbon sulfide. Halogenated hydrocarbons that have been in storage for extensive periods of time have the potential to degenerate due to the acidic nature of the halogen (chlorine), which can promote hydrogen transfer. This can create an environment promoting alkylation. Alkylation increases hydrocarbon chain length and complexity, creating large molecular weights, or oxidation. This can increase hydrocarbon stability if storage is not maintained under a nitrogen blanket.

Complex hydrocarbons are less efficiently destroyed by thermal treatments such as incineration. Smoking problems can arise for sulfur-bearing compounds such as HD if the sulfur is embedded within the structure of high molecular weight residues created by hydrogen transfer or oxidation. In these cases, sulfur atoms are trapped in a reducing environment and begin smoking when oxygen is more readily available.

It is unlikely that smoking should be a significant problem for the thermal processing of agent HD. Alkylation is more likely to initiate when the chemical structure is dominated with unsaturated compounds containing multiple bonds. These same multiple bonds also assist oxidation. Only the presence of significant quantities of impurities could create these conditions since HD does not contain any double or triple bonds. The simple, short chained structure of HD also does not favor the creation of excessively large chemical structures should alkylation occur.

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CONCLUSIONS AND RECOMMENDATIONS

Processing of HD ton containers having a combination of solid and liquid agent heels through the TOCDF MPF has been investigated for two temperature regimes. Vaporization curves for ton container center position solid heel depths varying from 1 inch to 7 inches, and having 2 inches of liquid agent over the solid heel, have been developed. The vaporization rate predictions were entered into mass and energy balance models to evaluate furnace operations while processing the ton containers at each of two furnace operating temperatures. All of the ton container cases investigated having solid heels and liquid agent over the top show that processing can be accomplished to 5X conditions well within permitted furnace operating conditions. Table 15 presents the recommended tray feed intervals and total furnace residence times required for processing of ton containers at 1,450°F with varying depths of solid agent heel. Table 16 presents these recommendations for the 1,600°F case. All cases were modeled with 2 inches of liquid agent over the solid heel.

Table 15: Summary of Tray Feed Interval and "5X" Minimum Residence Times for Furnace Operating at 1,450°F

	1-Inch Solid HD	2-Inch Solid HD	3-Inch Solid HD	4-Inch Solid HD	5-Inch Solid HD	6-Inch Solid HD	7-Inch Solid HD
Tray Feed Interval [minutes]	31	41	59	79	91	104	116
Minimum 5X Residence Time [minutes]	84	102	122	146	162	180	196

Table 16: Summary of Tray Feed Interval and "5X" Minimum Residence Times for Furnace Operating at 1,600°F

	1-Inch Solid HD	2-Inch Solid HD	3-Inch Solid HD	4-Inch Solid HD	5-Inch Solid HD	6-Inch Solid HD	7-Inch Solid HD
Tray Feed Interval [minutes]	24	36	52	67	77	88	98
Minimum 5X Residence Time [minutes]	72	86	106	122	136	152	164

It is recommended that the water spray nozzles in the top of furnace Zones 1 and 2 be changed to a vertical downward orientation in order to aid in furnace temperature control during processing of the HD ton containers.

Smoking as they exit from the discharge airlock is not anticipated to be a problem for ton containers with HD agent.

CONTINENTAL RESEARCH and Engineering, LLC
9785 S. Maroon Circle, Suite 100 Englewood, CO 80112 Phone (303) 758-7373 Fax (303) 758-1072

Appendix A

Ton Container Vaporization Rate Data

(MPF Operating Temperature 1,450°F)

CONTINENTAL RESEARCH and Engineering, LLC
9785 S. Maroon Circle, Suite 100 Englewood, CO 80112 Phone (303) 758-7373 Fax (303) 758-1072

Vaporization Rate Data for HD Ton Containers with Varying Solid Agent Heels and 2 Inches of Liquid Agent (MPF @ 1,450°F)

Elapsed Time (min)	Total Vaporization Rate (lbm/hr)						
	1" Solid +2" Liquid	2" Solid +2" Liquid	3" Solid +2" Liquid	4" Solid +2" Liquid	5" Solid +2" Liquid	6" Solid + Liquid	7" Solid +2" Liquid
0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	0.00	0.00	0.00	0.00	0.00	0.00	0.00
18	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	0.00	0.00	0.00	0.00	0.00	0.00	0.00
22	0.00	0.00	0.00	0.00	0.00	0.00	0.00
23	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	0.00	0.00	0.00	0.00	0.00	0.00	0.00
25	0.00	0.00	0.00	0.00	0.00	0.00	0.00
26	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	0.00	0.00	0.00	0.00	0.00	0.00	0.00
31	76.03	0.00	0.00	0.00	0.00	0.00	0.00
32	127.46	0.00	0.00	0.00	0.00	0.00	0.00
33	162.73	0.00	0.00	0.00	0.00	0.00	0.00
34	243.15	191.13	0.00	0.00	0.00	0.00	0.00
35	262.90	237.58	0.00	0.00	0.00	0.00	0.00
36	291.11	247.35	0.00	0.00	0.00	0.00	0.00
37	267.48	328.87	120.95	0.00	0.00	0.00	0.00
38	256.40	318.63	194.59	0.00	0.00	0.00	0.00
39	270.79	312.18	229.86	0.00	0.00	0.00	0.00
40	261.91	282.07	339.15	152.82	0.00	0.00	0.00

Vaporization Rate Data for HD Ton Containers with Varying Solid Agent Heels and 2 Inches of Liquid Agent (MPF @ 1,450°F)

Elapsed Time (min)	Total Vaporization Rate (lbm/hr)						
	1" Solid +2" Liquid	2" Solid +2" Liquid	3" Solid +2" Liquid	4" Solid +2" Liquid	5" Solid +2" Liquid	6" Solid + Liquid	7" Solid +2" Liquid
41	288.77	275.61	383.23	243.82	0.00	0.00	0.00
42	276.12	308.23	396.80	281.14	0.00	0.00	0.00
43	214.78	319.59	402.24	381.35	177.52	0.00	0.00
44	292.17	326.55	359.32	418.03	279.05	0.00	0.00
45	286.86	318.17	351.90	445.01	317.08	0.00	0.00
46	294.52	302.34	388.82	463.41	379.65	0.00	0.00
47	211.36	265.02	376.23	452.84	514.60	201.10	0.00
48	293.78	329.08	413.22	414.48	513.36	313.24	0.00
49	283.44	347.40	368.54	421.39	525.26	355.27	0.00
50	261.83	331.95	383.04	468.62	508.79	409.45	0.00
51	184.13	258.62	379.43	443.65	467.88	559.80	0.00
52	253.11	300.02	439.12	463.21	489.63	558.00	227.69
53	256.11	312.99	404.35	408.87	512.92	570.01	349.70
54	214.17	323.35	398.99	406.45	503.34	567.00	394.69
55	237.42	283.51	364.15	470.02	518.67	506.50	471.84
56	205.67	272.64	398.57	470.87	442.23	523.99	601.27
57	152.65	310.71	390.78	459.53	437.27	555.68	569.18
58	151.72	310.71	354.36	392.01	526.53	556.55	610.22
59	135.89	268.53	357.98	403.94	531.75	550.07	590.17
60	76.64	259.44	378.42	453.66	499.71	492.90	602.13
61	13.43	278.11	341.36	463.83	443.03	480.08	577.47
62	1.00	272.59	316.21	442.51	449.23	563.23	613.37
63	0.00	229.07	318.54	409.46	505.00	579.49	598.35
64		215.99	345.43	433.63	471.58	528.94	592.49
65		253.05	331.45	413.91	475.52	454.94	548.67
66		233.97	286.91	400.53	462.19	487.78	531.57
67		171.13	326.96	406.25	452.92	536.06	613.50
68		202.57	318.52	407.22	462.79	527.32	614.80
69		193.50	312.64	410.95	422.91	506.30	554.12
70		175.36	291.06	376.60	461.49	514.25	502.45
71		128.17	279.33	372.04	435.29	481.54	532.35
72		127.27	293.67	377.65	436.20	487.45	569.86
73		123.09	277.97	378.82	421.06	499.20	575.93
74		88.87	266.91	334.11	404.62	479.05	551.73
75		40.20	236.96	349.52	432.38	477.00	537.86
76		0.72	262.52	351.19	407.22	479.62	521.65
77		0.00	240.73	339.89	380.10	431.50	540.68
78			218.97	320.40	403.51	464.42	524.75
79			214.58	339.35	393.74	467.49	534.86
80			211.54	329.26	379.08	434.11	517.62

CONTINENTAL RESEARCH and Engineering, LLC
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Vaporization Rate Data for HD Ton Containers with Varying Solid Agent Heels and 2 Inches of Liquid Agent (MPF @ 1,450°F)

Elapsed Time (min)	Total Vaporization Rate (lbm/hr)						
	1" Solid +2" Liquid	2" Solid +2" Liquid	3" Solid +2" Liquid	4" Solid +2" Liquid	5" Solid +2" Liquid	6" Solid + Liquid	7" Solid +2" Liquid
81			204.24	321.38	366.49	415.65	494.49
82			195.59	294.50	363.32	433.33	499.41
83			174.23	300.46	374.64	425.19	500.80
84			169.75	305.61	352.86	421.69	489.19
85			164.36	285.30	346.97	402.05	483.42
86			153.60	266.69	325.63	393.21	456.85
87			139.05	273.20	335.64	392.90	476.44
88			122.72	277.86	336.49	402.45	468.72
89			124.32	266.80	314.37	373.88	456.16
90			106.96	243.87	312.36	374.29	432.15
91			73.47	247.57	307.35	368.93	440.30
92			56.79	243.20	291.24	363.20	436.38
93			38.84	239.20	299.91	356.84	436.12
94			6.34	222.80	287.31	352.99	421.31
95			0.00	228.36	291.78	337.59	401.17
96				216.43	267.06	332.23	409.23
97				213.43	278.85	331.03	414.41
98				202.79	265.13	329.85	386.88
99				189.15	275.86	323.97	384.42
100				182.91	263.42	322.88	385.46
101				181.89	263.57	302.36	371.71
102				164.54	243.05	312.40	373.42
103				156.32	246.79	313.83	371.74
104				154.50	251.68	302.01	363.82
105				134.68	242.40	299.54	344.80
106				126.36	229.78	293.21	354.30
107				114.90	220.94	278.08	342.53
108				105.05	223.93	300.68	335.45
109				88.07	203.88	273.54	340.12
110				70.88	200.87	278.16	323.19
111				57.07	184.14	270.10	316.76
112				45.76	187.98	271.88	330.52
113				32.10	167.39	250.36	320.51
114				13.88	159.64	264.28	311.49
115				1.15	146.63	251.04	308.94
116				0.00	135.84	231.55	308.40
117					131.47	240.67	311.49
118					123.06	229.50	309.02
119					122.18	221.16	307.77
120					108.27	224.39	291.27

Vaporization Rate Data for HD Ton Containers with Varying Solid Agent Heels and 2 Inches of Liquid Agent (MPF @ 1,450°F)

Elapsed Time (min)	Total Vaporization Rate (lbm/hr)						
	1" Solid +2" Liquid	2" Solid +2" Liquid	3" Solid +2" Liquid	4" Solid +2" Liquid	5" Solid +2" Liquid	6" Solid + Liquid	7" Solid +2" Liquid
121					96.02	198.23	283.99
122					89.85	209.16	296.08
123					77.89	187.35	277.13
124					63.86	198.47	276.58
125					49.39	175.01	270.55
126					39.80	173.68	247.00
127					24.46	155.47	255.30
128					12.79	162.15	246.78
129					0.50	145.22	227.80
130					0.00	148.82	235.72
131						128.95	215.77
132						127.48	225.19
133						116.52	213.55
134						112.94	207.66
135						101.24	201.34
136						84.97	198.41
137						74.89	197.17
138						66.72	186.03
139						55.45	180.43
140						45.85	171.16
141						34.30	164.49
142						25.33	157.42
143						15.41	150.86
144						2.29	134.34
145						0.00	124.99
146							119.97
147							111.84
148							94.18
149							97.19
150							87.79
151							79.32
152							68.66
153							57.19
154							46.53
155							35.57
156							23.77
157							18.01
158							9.90
159							0.69
160							0.00

CONTINENTAL RESEARCH and Engineering, LLC
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Appendix B

Ton Container Vaporization Rate Data

(MPF Operating Temperature 1,600°F)

CONTINENTAL RESEARCH and Engineering, LLC
9785 S. Maroon Circle, Suite 100 Englewood, CO 80112 Phone (303) 758-7373 Fax (303) 758-1072

Vaporization Rate Data for HD Ton Containers with Varying Solid Agent Heels and 2 Inches of Liquid Agent (MPF @ 1,600°F)

Elapsed Time (min)	Total Vaporization Rate (lbm/hr)						
	1" Solid +2" Liquid	2" Solid +2" Liquid	3" Solid +2" Liquid	4" Solid +2" Liquid	5" Solid +2" Liquid	6" Solid + Liquid	7" Solid +2" Liquid
0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16	0.00	0.00	0.00	0.00	0.00	0.00	0.00
17	0.00	0.00	0.00	0.00	0.00	0.00	0.00
18	0.00	0.00	0.00	0.00	0.00	0.00	0.00
19	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	0.00	0.00	0.00	0.00	0.00	0.00	0.00
22	0.00	0.00	0.00	0.00	0.00	0.00	0.00
23	0.00	0.00	0.00	0.00	0.00	0.00	0.00
24	0.00	0.00	0.00	0.00	0.00	0.00	0.00
25	0.00	0.00	0.00	0.00	0.00	0.00	0.00
26	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	0.00	0.00	0.00	0.00	0.00	0.00	0.00
28	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	0.00	0.00	0.00	0.00	0.00	0.00	0.00
30	0.00	0.00	0.00	0.00	0.00	0.00	0.00
31	76.03	0.00	0.00	0.00	0.00	0.00	0.00
32	127.46	0.00	0.00	0.00	0.00	0.00	0.00
33	162.73	0.00	0.00	0.00	0.00	0.00	0.00
34	243.15	191.13	0.00	0.00	0.00	0.00	0.00
35	262.90	237.58	0.00	0.00	0.00	0.00	0.00
36	291.11	247.35	0.00	0.00	0.00	0.00	0.00
37	267.48	328.87	120.95	0.00	0.00	0.00	0.00
38	256.40	318.63	194.59	0.00	0.00	0.00	0.00
39	270.79	312.18	229.86	0.00	0.00	0.00	0.00
40	261.91	282.07	339.15	152.82	0.00	0.00	0.00

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Vaporization Rate Data for HD Ton Containers with Varying Solid Agent Heels and 2 Inches of Liquid Agent (MPF @ 1,600°F)

Elapsed Time (min)	Total Vaporization Rate (lbm/hr)						
	1" Solid +2" Liquid	2" Solid +2" Liquid	3" Solid +2" Liquid	4" Solid +2" Liquid	5" Solid +2" Liquid	6" Solid + Liquid	7" Solid +2" Liquid
41	288.77	275.61	383.23	243.82	0.00	0.00	0.00
42	276.12	308.23	396.80	281.14	0.00	0.00	0.00
43	214.78	319.59	402.24	381.35	177.52	0.00	0.00
44	292.17	326.55	359.32	418.03	279.05	0.00	0.00
45	286.86	318.17	351.90	445.01	317.08	0.00	0.00
46	294.52	302.34	388.82	463.41	379.65	0.00	0.00
47	211.36	265.02	376.23	452.84	514.60	201.10	0.00
48	293.78	329.08	413.22	414.48	513.36	313.24	0.00
49	283.44	347.40	368.54	421.39	525.26	355.27	0.00
50	261.83	331.95	383.04	468.62	508.79	409.45	0.00
51	184.13	258.62	379.43	443.65	467.88	559.80	0.00
52	253.11	300.02	439.12	463.21	489.63	558.00	227.69
53	256.11	312.99	404.35	408.87	512.92	570.01	349.70
54	214.17	323.35	398.99	406.45	503.34	567.00	394.69
55	237.42	283.51	364.15	470.02	518.67	506.50	471.84
56	205.67	272.64	398.57	470.87	442.23	523.99	601.27
57	152.65	310.71	390.78	459.53	437.27	555.68	569.18
58	151.72	310.71	354.36	392.01	526.53	556.55	610.22
59	135.89	268.53	357.98	403.94	531.75	550.07	590.17
60	76.64	259.44	378.42	453.66	499.71	492.90	602.13
61	13.43	278.11	341.36	463.83	443.03	480.08	577.47
62	1.00	272.59	316.21	442.51	449.23	563.23	613.37
63	0.00	229.07	318.54	409.46	505.00	579.49	598.35
64		215.99	345.43	433.63	471.58	528.94	592.49
65		253.05	331.45	413.91	475.52	454.94	548.67
66		233.97	286.91	400.53	462.19	487.78	531.57
67		171.13	326.96	406.25	452.92	536.06	613.50
68		202.57	318.52	407.22	462.79	527.32	614.80
69		193.50	312.64	410.95	422.91	506.30	554.12
70		175.36	291.06	376.60	461.49	514.25	502.45
71		128.17	279.33	372.04	435.29	481.54	532.35
72		127.27	293.67	377.65	436.20	487.45	569.86
73		123.09	277.97	378.82	421.06	499.20	575.93
74		88.87	266.91	334.11	404.62	479.05	551.73
75		40.20	236.96	349.52	432.38	477.00	537.86
76		0.72	262.52	351.19	407.22	479.62	521.65
77		0.00	240.73	339.89	380.10	431.50	540.68
78			218.97	320.40	403.51	464.42	524.75
79			214.58	339.35	393.74	467.49	534.86
80			211.54	329.26	379.08	434.11	517.62

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Vaporization Rate Data for HD Ton Containers with Varying Solid Agent Heels and 2 Inches of Liquid Agent (MPF @ 1,600°F)

Elapsed Time (min)	Total Vaporization Rate (lbm/hr)						
	1" Solid +2" Liquid	2" Solid +2" Liquid	3" Solid +2" Liquid	4" Solid +2" Liquid	5" Solid +2" Liquid	6" Solid + Liquid	7" Solid +2" Liquid
81			204.24	321.38	366.49	415.65	494.49
82			195.59	294.50	363.32	433.33	499.41
83			174.23	300.46	374.64	425.19	500.80
84			169.75	305.61	352.86	421.69	489.19
85			164.36	285.30	346.97	402.05	483.42
86			153.60	266.69	325.63	393.21	456.85
87			139.05	273.20	335.64	392.90	476.44
88			122.72	277.86	336.49	402.45	468.72
89			124.32	266.80	314.37	373.88	456.16
90			106.96	243.87	312.36	374.29	432.15
91			73.47	247.57	307.35	368.93	440.30
92			56.79	243.20	291.24	363.20	436.38
93			38.84	239.20	299.91	356.84	436.12
94			6.34	222.80	287.31	352.99	421.31
95			0.00	228.36	291.78	337.59	401.17
96				216.43	267.06	332.23	409.23
97				213.43	278.85	331.03	414.41
98				202.79	265.13	329.85	386.88
99				189.15	275.86	323.97	384.42
100				182.91	263.42	322.88	385.46
101				181.89	263.57	302.36	371.71
102				164.54	243.05	312.40	373.42
103				156.32	246.79	313.83	371.74
104				154.50	251.68	302.01	363.82
105				134.68	242.40	299.54	344.80
106				126.36	229.78	293.21	354.30
107				114.90	220.94	278.08	342.53
108				105.05	223.93	300.68	335.45
109				88.07	203.88	273.54	340.12
110				70.88	200.87	278.16	323.19
111				57.07	184.14	270.10	316.76
112				45.76	187.98	271.88	330.52
113				32.10	167.39	250.36	320.51
114				13.88	159.64	264.28	311.49
115				1.15	146.63	251.04	308.94
116				0.00	135.84	231.55	308.40
117					131.47	240.67	311.49
118					123.06	229.50	309.02
119					122.18	221.16	307.77
120					108.27	224.39	291.27

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Vaporization Rate Data for HD Ton Containers with Varying Solid Agent Heels and 2 Inches of Liquid Agent (MPF @ 1,600°F)

Elapsed Time (min)	Total Vaporization Rate (lbm/hr)						
	1" Solid +2" Liquid	2" Solid +2" Liquid	3" Solid +2" Liquid	4" Solid +2" Liquid	5" Solid +2" Liquid	6" Solid + Liquid	7" Solid +2" Liquid
121					96.02	198.23	283.99
122					89.85	209.16	296.08
123					77.89	187.35	277.13
124					63.86	198.47	276.58
125					49.39	175.01	270.55
126					39.80	173.68	247.00
127					24.46	155.47	255.30
128					12.79	162.15	246.78
129					0.50	145.22	227.80
130					0.00	148.82	235.72
131						128.95	215.77
132						127.48	225.19
133						116.52	213.55
134						112.94	207.66
135						101.24	201.34
136						84.97	198.41
137						74.89	197.17
138						66.72	186.03
139						55.45	180.43
140						45.85	171.16
141						34.30	164.49
142						25.33	157.42
143						15.41	150.86
144						2.29	134.34
145						0.00	124.99
146							119.97
147							111.84
148							94.18
149							97.19
150							87.79
151							79.32
152							68.66
153							57.19
154							46.53
155							35.57
156							23.77
157							18.01
158							9.90
159							0.69
160							0.00